EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S1	226	(564/510).CCLS.	US-PGPUB; USPAT; EPO; DERWENT	OR	OFF	2006/11/02 11:05
S2	16	(("2859245") or ("3092637") or ("3213062") or ("3061631") or ("3214428")).PN.	US-PGPUB; USPAT; EPO; DERWENT	OR	OFF	2006/11/02 11:12
S3	4	(("6235939") or ("6184425")).PN.	US-PGPUB; USPAT; EPO; DERWENT	OR	OFF	2006/11/02 11:11
S4	19	(("3221007") or ("3976691") or ("4497937") or ("6080886") or ("6222064") or ("6329529") or ("6458990") or ("6632949") or ("3899496") or ("4925939")).PN.	US-PGPUB; USPAT; EPO; DERWENT	OR	OFF	2006/11/02 11:13
S5	3	(("20020042521") or ("20030004348")).PN.	US-PGPUB; USPAT; EPO; DERWENT	OR	OFF	2006/11/02 11:13

```
Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSSPTA1600RXA

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  AUG 09   INSPEC enhanced with 1898-1968 archive
 NEWS  4  AUG 28   ADISCTI Reloaded and Enhanced
 NEWS  5  AUG 30   CA(SM)/CAplus(SM) Austrian patent law changes
 NEWS  6  SEP 11   CA/CAplus enhanced with more pre-1907 records
 NEWS  7  SEP 21   CA/CAplus fields enhanced with simultaneous left and right
                   truncation
 NEWS  8  SEP 25   CA(SM)/CAplus(SM) display of CA Lexicon enhanced
 NEWS  9  SEP 25   CAS REGISTRY(SM) no longer includes Concord 3D coordinates
 NEWS 10  SEP 25   CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
 NEWS 11  SEP 28   CEABA-VTB classification code fields reloaded with new
                   classification scheme
 NEWS 12  OCT 19   LOGOFF HOLD duration extended to 120 minutes
 NEWS 13  OCT 19   E-mail format enhanced
 NEWS 14  OCT 23   Option to turn off MARPAT highlighting enhancements available
 NEWS 15  OCT 23   CAS Registry Number crossover limit increased to 300,000 in
                   multiple databases
 NEWS 16  OCT 23   The Derwent World Patents Index suite of databases on STN
                   has been enhanced and reloaded
 NEWS 17  OCT 30   CHEMLIST enhanced with new search and display field

 NEWS EXPRESS  JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:19:43 ON 02 NOV 2006

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.21       0.21
```

FILE 'REGISTRY' ENTERED AT 09:19:58 ON 02 NOV 2006

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 NOV 2006 HIGHEST RN 912260-33-4
DICTIONARY FILE UPDATES: 1 NOV 2006 HIGHEST RN 912260-33-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

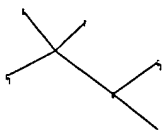
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

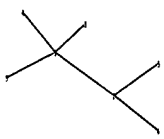
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\10751623.str





chain nodes :
1 2 3 4 5 6 9
chain bonds :
1-2 1-3 1-4 1-9 2-5 2-6

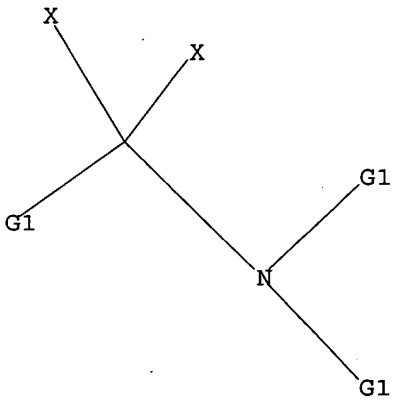
exact/norm bonds :
1-2 1-9 2-5 2-6
exact bonds :
1-3 1-4

G1:C,H

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:CLASS

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:33:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1001 TO ITERATE

100.0% PROCESSED   1001 ITERATIONS   50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 18122 TO   21918
PROJECTED ANSWERS: 800 TO   1760

L2   50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:33:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   21588 TO ITERATE

100.0% PROCESSED   21588 ITERATIONS   1526 ANSWERS
SEARCH TIME: 00.00.01

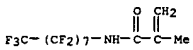
L3   1526 SEA SSS FUL L1

```
=> s l3 and caplus/lc
      52542643 CAPLUS/LC
L4         1268 L3 AND CAPLUS/LC

=> s l3 not l4
L5          258 L3 NOT L4

=> d l5 200
```

L5 ANSWER 200 OF 258 REGISTRY COPYRIGHT 2006 ACS on STN
RN 150625-14-2 REGISTRY
ED Entered STN: 14 Oct 1993
CN 2-Propenamide, N-(heptadecafluorooctyl)-2-methyl- (9CI) (CA INDEX NAME)
MF C12 H6 F17 N O
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
=> fil caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       185.04     185.25

FILE 'CAPLUS' ENTERED AT 09:36:18 ON 02 NOV 2006
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FILE COVERS 1907 - 2 Nov 2006  VOL 145 ISS 19
FILE LAST UPDATED: 1 Nov 2006  (20061101/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l4
L6         2413 L4

=> fil stnguide
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.46     185.71

FILE 'STNGUIDE' ENTERED AT 09:36:24 ON 02 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 27, 2006 (20061027/UP).

=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.06     185.77

FILE 'REGISTRY' ENTERED AT 09:36:53 ON 02 NOV 2006
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COPYRIGHT (C) 2006 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES:     1 NOV 2006  HIGHEST RN 912260-33-4
DICTIONARY FILE UPDATES:    1 NOV 2006  HIGHEST RN 912260-33-4
```

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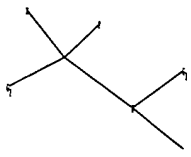
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

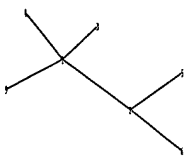
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\10751623.str





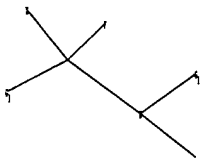
chain nodes :
1 2 3 4 5 6 9
chain bonds :
1-2 1-3 1-4 1-9 2-5 2-6
exact/norm bonds :
1-2 1-9 2-5 2-6
exact bonds :
1-3 1-4

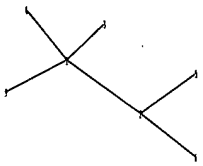
G1:C,H

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:CLASS

L7 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\10751623.str





chain nodes :
1 2 3 4 5 6 9
chain bonds :
1-2 1-3 1-4 1-9 2-5 2-6
exact/norm bonds :
1-2 1-9 2-5 2-6
exact bonds :
1-3 1-4

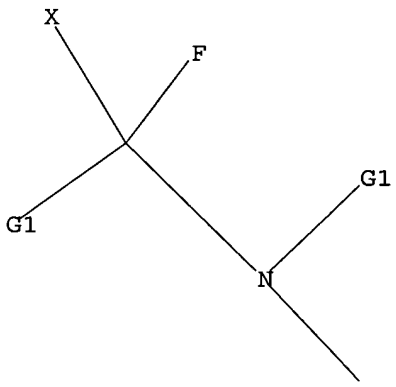
G1:C,H

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:CLASS

L8   STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8   STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> d his

     (FILE 'HOME' ENTERED AT 09:19:43 ON 02 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 09:19:58 ON 02 NOV 2006
L1   STRUCTURE UPLOADED
L2   50 S L1
L3   1526 S L1 FULL
L4   1268 S L3 AND CAPLUS/LC
L5   258 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:36:18 ON 02 NOV 2006
L6   2413 S L4

     FILE 'STNGUIDE' ENTERED AT 09:36:24 ON 02 NOV 2006

     FILE 'REGISTRY' ENTERED AT 09:36:53 ON 02 NOV 2006
L7   STRUCTURE UPLOADED
L8   STRUCTURE UPLOADED

=> s l8 subset=l3 full
FULL SUBSET SEARCH INITIATED 09:37:47 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -   1220 TO ITERATE

100.0% PROCESSED   1220 ITERATIONS   1139 ANSWERS
SEARCH TIME: 00.00.01

```
L9          1139 SEA SUB=L3 SSS FUL L8

=> s l9 and caplus/lc
      52542643 CAPLUS/LC
L10          972 L9 AND CAPLUS/LC

=> s l9 not l10
L11          167 L9 NOT L10

=> d l11 100
```

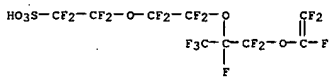
L11 ANSWER 100 OF 167 REGISTRY COPYRIGHT 2006 ACS on STN
RN 339995-57-2 REGISTRY
ED Entered STN: 07 Jun 2001
CN Ethanesulfonic acid, 2-[2-[1-[difluoro[(trifluoroethenyl)oxy]methyl]-

1,2,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoro-
, compd. with 1,1,2,2,2-pentafluoro-N,N-bis(pentafluoroethyl)ethanamine
(1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanamine, 1,1,2,2,2-pentafluoro-N,N-bis(pentafluoroethyl)-,

2-[2-[1-[difluoro[(trifluoroethenyl)oxy]methyl]-1,2,2,2-tetrafluoroethoxy]-
1,1,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoroethanesulfonate (9CI)
MF C9 H F17 O6 S . C6 F15 N
CI COM
SR CA

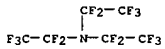
CM 1

CRN 339995-56-1
CMF C9 H F17 O6 S



CM 2

CRN 359-70-6
CMF C6 F15 N

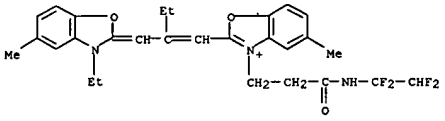


```
=> s l9 and 1-2/F
       1713397 1-2/F
L12          48 L9 AND 1-2/F

=> s l9 not l12
L13        1091 L9 NOT L12

=> d scan l13
```

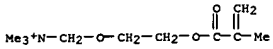
L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzoxazolium, 2-[2-[(3-ethyl-5-methyl-2(3H)-benzoxazolylidene)methyl]-1-butenyl]-5-methyl-3-[3-oxo-3-[(1,1,2,2-tetrafluoroethyl)amino]propyl]- (9CI)
MF C28 H30 F4 N3 O3
CI COM



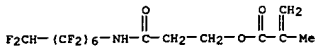
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Methanaminium, N,N,N-trimethyl-1-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethoxy]-, polymer with 3-oxo-3-[(1,1,2,2,3,3,4,4,5,5,6,6,7,7-tetradecafluoroheptyl)amino]propyl 2-methyl-2-propenoate (9CI)
MF (C14 H11 F14 N O3 . C10 H20 N O3)x
CI PMS

CM 1

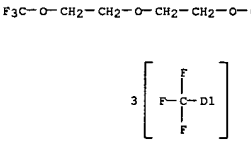


CM 2



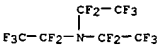
L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Propanesulfonic acid, hexafluoro-1(or 2)-[trifluoro(trifluoromethyl)-2-[trifluoro-2-(trifluoromethoxy)(trifluoromethyl)ethoxy]ethoxy]-, compd. with 1,1,2,2,2-pentafluoro-N,N-bis(pentafluoroethyl)ethanamine (1:1) (9CI)
MF C10 H F21 O6 S . C6 F15 N

CM 1

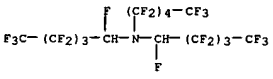


9 (D1—F)

CM 2

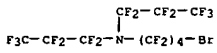


L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Pentanamine, N,N-bis(1,2,2,3,3,4,4,5,5,5-decafluoropentyl)-1,1,2,2,3,3,4,4,5,5,5-undecafluoro- (9CI)
MF C15 H2 F31 N



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

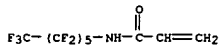
L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Butanamine, 4-bromo-1,1,2,2,3,3,4,4-octafluoro-N,N-bis(heptafluoropropyl)- (9CI)
MF C10 Br F22 N



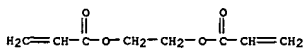
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenoic acid, 1,2-ethanediyl ester, polymer with butyl 2-propenoate and N-(tridecafluorohexyl)-2-propenamide, graft (9CI)
MF (C9 H4 F13 N O . C8 H10 O4 . C7 H12 O2)x
CI PMS

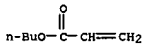
CM 1



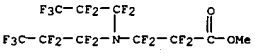
CM 2



CM 3



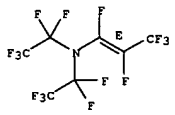
L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Propanoic acid, 3-[bis(heptafluoropropyl)amino]-2,2,3,3-tetrafluoro-, methyl ester (9CI)
MF C10 H3 F18 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

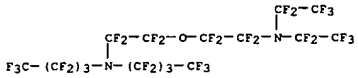
L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Propen-1-amine, 1,2,3,3,3-pentafluoro-N,N-bis(pentafluoroethyl)-, (E)- (9CI)
MF C7 F15 N

Double bond geometry as shown.



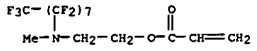
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Butanamine, N-[2-[2-(bis(pentafluoroethyl)amino]-1,1,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoroethyl]-1,1,2,2,3,3,4,4,4-nonafluoro-N-(nonafluorobutyl)- (9CI)
MF C16 F36 N2 O



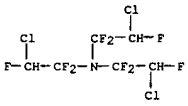
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenoic acid, 2-[(heptadecafluorooctyl)methylamino]ethyl ester (9CI)
MF C14 H10 F17 N O2
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 1091 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Ethanamine, 2-chloro-N,N-bis(2-chloro-1,1,2-trifluoroethyl)-1,1,2-trifluoro- (9CI)
MF C6 H3 Cl3 F9 N



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> d his

     (FILE 'HOME' ENTERED AT 09:19:43 ON 02 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 09:19:58 ON 02 NOV 2006
L1             STRUCTURE UPLOADED
L2              50 S L1
L3            1526 S L1 FULL
L4            1268 S L3 AND CAPLUS/LC
L5             258 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:36:18 ON 02 NOV 2006
L6            2413 S L4

     FILE 'STNGUIDE' ENTERED AT 09:36:24 ON 02 NOV 2006

     FILE 'REGISTRY' ENTERED AT 09:36:53 ON 02 NOV 2006
L7             STRUCTURE UPLOADED
L8             STRUCTURE UPLOADED
L9            1139 S L8 FULL SUB=L3
L10            972 S L9 AND CAPLUS/LC
L11            167 S L9 NOT L10
L12             48 S L9 AND 1-2/F
L13           1091 S L9 NOT L12

=> d scan l12
```

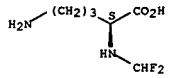
L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Formamide, N-(difluoromethyl)- (9CI)
MF C2 H3 F2 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

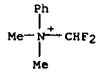
L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN L-Ornithine, N2-(difluoromethyl)- (9CI)
MF C6 H12 F2 N2 O2

Absolute stereochemistry.



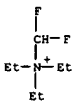
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenaminium, N-(difluoromethyl)-N,N-dimethyl- (9CI)
MF C9 H12 F2 N
CI COM



L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Ethanaminium, N-(difluoromethyl)-N,N-diethyl-, sulfite (1:1) (9CI)
MF C7 H16 F2 N . H O3 S

CM 1



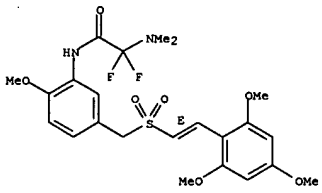
CM 2

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI)
MF C3 H7 F2 N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Acetamide, 2-(dimethylamino)-2,2-difluoro-N-[2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl]methyl]phenyl]- (9CI)
MF C23 H28 F2 N2 O7 S

Double bond geometry as shown.

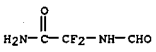


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Propanamine, N-(2,2-dichloro-1,1-difluoroethyl)-N-propyl- (9CI)
MF C8 H15 Cl2 F2 N

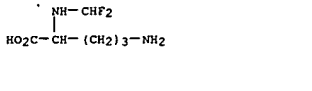
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Acetamide, 2,2-difluoro-2-(formylamino)- (9CI)
MF C3 H4 F2 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Ornithine, N2-(difluoromethyl)-, monohydrochloride (9CI)
MF C6 H12 F2 N2 O2 . Cl H



L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Carbamic acid, (1,1-difluoroethyl)-, ethyl ester (9CI)
MF C5 H9 F2 N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Acetyl chloride, (dimethylamino)difluoro- (9CI)
MF C4 H6 Cl F2 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> d his

     (FILE 'HOME' ENTERED AT 09:19:43 ON 02 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 09:19:58 ON 02 NOV 2006
L1             STRUCTURE UPLOADED
L2              50 S L1
L3            1526 S L1 FULL
L4            1268 S L3 AND CAPLUS/LC
L5             258 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:36:18 ON 02 NOV 2006
L6            2413 S L4

     FILE 'STNGUIDE' ENTERED AT 09:36:24 ON 02 NOV 2006

     FILE 'REGISTRY' ENTERED AT 09:36:53 ON 02 NOV 2006
L7             STRUCTURE UPLOADED
L8             STRUCTURE UPLOADED
L9            1139 S L8 FULL SUB=L3
L10            972 S L9 AND CAPLUS/LC
L11            167 S L9 NOT L10
L12             48 S L9 AND 1-2/F
L13           1091 S L9 NOT L12

=> s l12 and caplus/lc
      52542643 CAPLUS/LC
L14           41 L12 AND CAPLUS/LC

=> s l12 not l14
L15            7 L12 NOT L14
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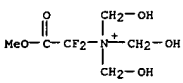
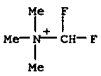
L15 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 884233-01-6 REGISTRY
ED Entered STN: 15 May 2006
CN Ethanaminium, 1,1-difluoro-N,N,N-tris(hydroxymethyl)-2-methoxy-2-oxo- (9CI) (CA INDEX NAME)
MF C6 H12 F2 N O5
SR Chemical Library
Supplier: AKos Consulting and Solutions GmbH
LC STN Files: CHEMCATS



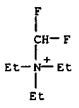
L15 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 788118-27-4 REGISTRY
ED Entered STN: 24 Nov 2004
CN Benzenaminium, N-(difluoromethyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)
MF C9 H12 F2 N
CI COM
SR CA

L15 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 756779-19-8 REGISTRY
ED Entered STN: 04 Oct 2004
CN Ethanaminium, N-(difluoromethyl)-N-ethyl-N-methyl- (9CI) (CA INDEX NAME)
MF C6 H14 F2 N
CI COM
SR CA

L15 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 729552-22-1 REGISTRY
ED Entered STN: 21 Aug 2004
CN Methanaminium, 1,1-difluoro-N,N,N-trimethyl- (9CI) (CA INDEX NAME)
MF C4 H10 F2 N
CI COM
SR CA



L15 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 124462-77-7 REGISTRY
ED Entered STN: 29 Dec 1989
CN Ethanaminium, N-(difluoromethyl)-N,N-diethyl- (9CI) (CA INDEX NAME)
MF C7 H16 F2 N
CI COM
SR CA



L15 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 663-75-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethanamine, 2,2-dichloro-1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethylamine, 2,2-dichloro-1,1-difluoro-N,N-dimethyl- (6CI, 8CI)
MF C4 H7 Cl2 F2 N
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)

$Me_2N-CF_2-CHCl_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L15 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 646-56-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethylamine, 1,1-difluoro-N,N-dimethyl- (6CI, 8CI)
MF C4 H9 F2 N
LC STN Files: CAOLD

$Me-CF_2-NMe_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	72.40	258.17

FILE 'CAPLUS' ENTERED AT 09:41:55 ON 02 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 2 Nov 2006 VOL 145 ISS 19
FILE LAST UPDATED: 1 Nov 2006 (20061101/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> d his

=> d ibib abs hitstr 1-49

L16 ANSWER 1 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:75198 CAPLUS
DOCUMENT NUMBER: 144:177462
TITLE: Parenteral formulations of (E)-2,6-dialkoxystyryl 4-substituted benzylsulfones for treatment of abnormal cell proliferation
INVENTOR(S): Bell, Staneley C.; Wong, Albert; Maniar, Manoj
PATENT ASSIGNEE(S): Onconova Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006010152	A2	20060126	WO 2005-US25224	20050715
WO 2006010152	A3	20060908		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-589075P P 20040719

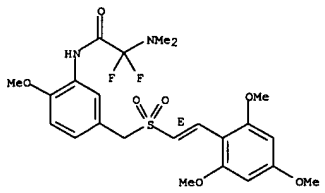
OTHER SOURCE(S): MARPAT 144:177462

AB Parenteral formulations are provided comprising (i) amino substituted (E)-2,6-dialkoxystyryl 4-substituted benzylsulfones and the sodium and potassium salts thereof, and (ii) at least about 50% by weight of at least one water-soluble polymer for the prevention and/or treatment of conditions mediated by abnormal cell proliferation. The water-soluble polymer is selected from polyethylene glycol (PEG), polyoxyethylene, polyoxyethylene-polyoxypropylene copolymers, polyglycerol, polyvinyl alc., polyvinylpyrrolidone (PVP), polyvinylpyridine N-oxide, and copolymer of vinylpyridine N-oxide and vinylpyridine. For example, (E)-2,4,6-trimethoxystyryl-3-[(carboxymethyl)amino]-4-methoxybenzylsulfone Na salt (ON 01910.Na, Novonex) was prepared and formulated into a stable parenteral solution containing Novonex 75 mg/mL and 50% PEG-400 in 0.016 M phosphate buffer, pH 10. Dilution of this product 1:7 with 0.00025 M phosphoric acid, for example, yielded a product that has a pH of about 7.4 and osmolarity of approx. 300 mOsm/kg.

IT 592543-18-5
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(parenteral formulations of dialkoxystyryl benzylsulfones containing water-soluble polymer for prevention and/or treatment of abnormal cell proliferation)

L16 ANSWER 1 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 592543-18-5 CAPLUS
CN Acetamide, 2-(dimethylamino)-2,2-difluoro-N-[2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L16 ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1049789 CAPLUS
DOCUMENT NUMBER: 143:346909
TITLE: Preparation of substituted phenoxy- and phenylthio-derivatives for treating proliferative disorders and as radioprotectants and chemoprotectants
INVENTOR(S): Reddy, E. Premkumar; Reddy, M. V. Ramana; Bell, Stanley C.
PATENT ASSIGNEE(S): Temple University-of the Commonwealth System of Higher Education, USA; Onconova Therapeutics Inc.
SOURCE: PCT Int. Appl., 179 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005089269	A2	20050929	WO 2005-US8429	20050315

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005222947	A1	20050929	AU 2005-222947	20050315

PRIORITY APPLN. INFO.: US 2004-554008P P 20040316
WO 2005-US8429 W 20050315

OTHER SOURCE(S): MARPAT 143:346909
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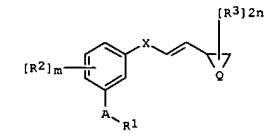
L16 ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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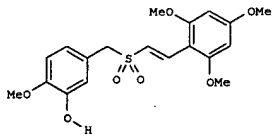


II

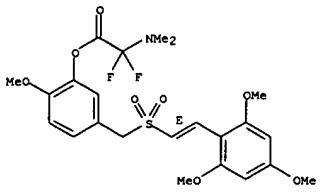
AB Title compds. I [A = S, O; R1 = H, haloalkyl, (un)substituted hetero/aryl, etc.; Q = hetero/aryl; R2, R3 = independently halo, hydrocarbyl, NO2, CN, OH and derivs., P(:O)(OH)2 and derivs., etc.; X = -NRX-Z-, -CH(Rx)Y-; Y = SO, SO2; Z = CO, SO2; Rx = H, alkyl, -CO-alkyl; with provisos; and their geometrical isomers] were prepared as antiproliferative agents including, for example, anticancer agents and as radioprotective and chemoprotective agents. For example, reacting 2-[(3-hydroxy-4-methoxybenzyl)sulfonyl]acetic acid with 2,4,6-Trimethoxybenzaldehyde in the presence of PhCO2H/piperidine/toluene for 2-3 h at reflux gave II in 62.5% yield.. I displayed antiproliferative activity; for II GI50 values = 0.004 μM, 0.001 μM, and 0.005 μM towards Sk-OV-3, RF-48, and CEM tumor cell lines, resp.

IT 865784-78-7P, (E)-5-[[(2,4,6-Trimethoxystyryl)sulfonyl]methyl]-2-methoxyphenyl 2-(dimethylamino)-2,2-difluoroacetate 865785-19-9P, (E)-5-[[(2,4,6-Trimethoxystyryl)sulfinyl]methyl]-2-methoxyphenyl 2-(dimethylamino)-2,2-difluoroacetate 865785-58-6P, 5-[[[(1E)-2-(2,4,6-Trimethoxyphenyl)ethenyl]sulfonyl]amino]-2-methoxyphenyl 2-(dimethylamino)-2,2-difluoroacetate 865785-95-1P, 5-[[[(E)-2-(2,4,6-Trimethoxyphenyl)ethenyl]carbonyl]amino]-2-methoxyphenyl 2-(dimethylamino)-2,2-difluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of substituted phenoxy- and phenylthio-derivs. for treating proliferative disorders and as radioprotectants and chemoprotectants)

RN 865784-78-7 CAPLUS
CN Acetic acid, (dimethylamino)difluoro-, 2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl]methyl]phenyl ester (9CI) (CA INDEX NAME)

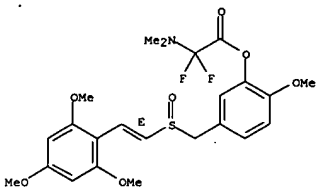
Double bond geometry as shown.

L16 ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



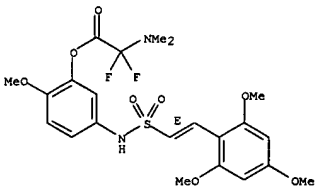
RN 865785-19-9 CAPLUS
CN Acetic acid, (dimethylamino)difluoro-, 2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfinyl]methyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 865785-58-6 CAPLUS
CN Acetic acid, (dimethylamino)difluoro-, 2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl]amino]phenyl ester (9CI) (CA INDEX NAME)

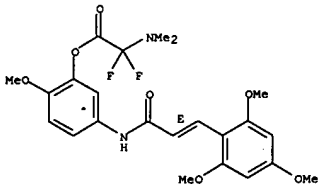
Double bond geometry as shown.



L16 ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 865785-95-1 CAPLUS
CN Acetic acid, (dimethylamino)difluoro-, 2-methoxy-5-[[(2E)-1-oxo-3-(2,4,6-trimethoxyphenyl)-2-propenyl]amino]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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ACCESSION NUMBER: 2005:611586 CAPLUS
DOCUMENT NUMBER: 143:117441
TITLE: Binary mixtures of 1,1,1,3,3-pentafluorobutane with hydrofluorocarbons, (difluoromethyl)dimethylamine, and (perfluoroethyl) Et sulfide as refrigerants and heat transfer fluids
INVENTOR(S): Minor, Barbara Haviland; Nappa, Mario J.; Sievert, Allen C.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005151111	A1	20050714	US 2004-14435	20041216
US 2005151113	A1	20050714	US 2004-14000	20041216
US 2005151112	A1	20050714	US 2004-14438	20041216
US 2005156135	A1	20050721	US 2004-13901	20041216
US 2005156138	A1	20050721	US 2004-14333	20041216
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US 2005156134	A1	20050721	US 2004-14334	20041216
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L16 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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L16 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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WO 2006012096 A1 20060202 WO 2005-US21800 20050621

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

WO 2006012097 A1 20060202 WO 2005-US21801 20050621

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

L16 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

US 2004-584785P P 20040629

US 2004-13901 A 20041216

US 2004-14000 A 20041216

US 2004-14006 A 20041216

US 2004-14333 A 20041216

US 2004-14334 A 20041216

US 2004-14343 A 20041216

US 2004-14435 A 20041216

US 2004-14438 A 20041216

WO 2005-US1504 W 20050112

WO 2005-US1505 W 20050112

WO 2005-US1506 W 20050112

WO 2005-US1507 W 20050112

WO 2005-US1508 W 20050112

WO 2005-US1509 W 20050112

WO 2005-US1510 W 20050112

WO 2005-US1511 W 20050112

US 2005-62975 A 20050222

US 2005-63040 A3 20050222

US 2005-63178 A 20050222

US 2005-63203 A3 20050222

US 2005-151481 A 20050613

US 2005-152731 A 20050614

US 2005-152732 A 20050614

US 2005-153168 A 20050615

US 2005-153195 A 20050615

US 2005-153804 A 20050615

OTHER SOURCE(S): MARPAT 143:117441

AB Refrigerant or heat transfer fluids are binary mixts. of 1,1,1,3,3-pentafluorobutane (HFC 365mfc) with hydrofluorocarbons, N-(difluoromethyl)-N,N-dimethylamine, and 1,1,1,2,2-pentafluoro-2-[(pentafluoroethyl)thio]ethane. Suitable hydrofluorocarbon co-refrigerants include 1,1,3-trifluoropropane, 1,3-difluoropropane,

L16 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,1-difluorobutane, 1,3-difluoro-2-methylpropane, 1,2-difluoro-2-methylpropane, 1,2-difluorobutane, 1,3-difluorobutane, 2,3-difluorobutane,
1,1,1-trifluoropentane, 1,1,1-trifluoro-3-methylbutane, and 1,2-difluoropentane, 3,3,4,4,5,5,6,6,6-nonafluoro-1-hexene. The compns., which have no ozone depletion potential and low global warming potential, are useful in centrifugal compressors, two-stage compressors, or single-pass heat exchangers. The compn. may also contain a UV-fluorescent
dye, a solubilizer (selected from a no. of compd. classes), and nitromethane thermal stabilizer. The binary mixts. are preferably binary azeotropes.

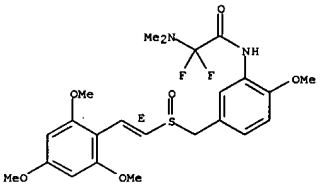
IT 683-81-8
RL: TEM (Technical or engineered material use); USES (Uses)
(mixts. with pentafluorobutane; binary mixts. of 1,1,1,3,3-pentafluorobutane with hydrofluorocarbons, (difluoromethyl)dimethylamine, and (perfluoroethyl) Et sulfide as refrigerants and heat transfer fluids)

RN 683-81-8 CAPLUS

CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 4 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
trimethoxyphenyl)ethenyl]sulfinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L16 ANSWER 4 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:451126 CAPLUS

DOCUMENT NUMBER: 143:1247

TITLE: α,β-Unsaturated sulfoxides for treating proliferative disorders and as radioprotective and chemoprotective agents

INVENTOR(S): Reddy, Premkumar E.; Reddy, Ramana M. V.; Bell, Stanley C.

PATENT ASSIGNEE(S): Temple University-of the Commonwealth System of Higher
Education, USA; Onconova Therapeutics Inc.

SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005046599	A2	20050526	WO 2004-US37293	20041108
WO 2005046599	A3	20051006		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004289281	A1	20050526	AU 2004-289281	20041108
CA 2546495	AA	20050526	CA 2004-2546495	20041108
EP 1689706	A2	20060816	EP 2004-816944	20041108
R: AT, BE, CH, LI, CY, BG, CZ				

PRIORITY APPLN. INFO.:	US 2003-520523P	P	20031114
	WO 2004-US37293	W	20041108

OTHER SOURCE(S): MARPAT 143:1247

AB αβ-Unsatd. sulfoxides Ar1[CH(R1)]nS(O)CH=CHAr2 [Ar1, Ar2 = (un)substituted (hetero)aryl (when Ar1 and Ar2 are both Ph, at least one of Ar1 and Ar2 is substituted); n = 0, 1; R1 = H, C1-8 hydrocarbyl, CN, etc.; conformation of substituents on carbon-carbon double bond is E or Z;
conformation of substituents on sulfoxide S atom is R-, S- or any mixture of
R- and S-; when R1 other than H, conformation of substituents on carbon atom to which R1 is attached is R-, S- or any mixture of R- and S-] are disclosed which are useful as antiproliferative agents including e.g. anticancer agents and as radioprotective and chemoprotective agents. Processes or preg. compds. of the invention are also disclosed.

IT 852283-73-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(α,β-unsatd. sulfoxides for treatment of proliferative disorders and as radioprotectants and chemoprotectants)

RN 852283-73-9 CAPLUS

CN Acetamide, 2-(dimethylamino)-2,2-difluoro-N-[2-methoxy-5-[[[(1E)-2-(2,4,6-

L16 ANSWER 5 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:630872 CAPLUS

DOCUMENT NUMBER: 142:198334

TITLE: Theoretical study of peptide model dimers. Homo versus
heterochiral complexes

AUTHOR(S): Alkorta, Ibon; Elguero, Jose

CORPORATE SOURCE: Instituto de Quimica Medica, CSIC, Madrid, E-28006, Spain

SOURCE: THEOCHEM (2004), 680(1-3), 191-198
CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The study of possible chiral recognition of a series of peptide models (For-Gly-NH2, For-Ala-NH2 and four of their fluoro substituted derivs.) has been carried out by means of DFT calcns. Homo (L,L) and heterochiral (L,D) dimers formed by hydrogen bond (HB) complexation have been considered. Initially, the conformational preferences of the monomers have been calculated and used to generate all the possible homo and heterochiral dimers. The energetic results show that in most cases, the β monomers are the most stable while in the dimers, the γ-γ complexes show the strongest interaction energies. In three of the four chiral cases studied, a heterochiral dimer is the most stable one. In addition, the electron d. and nuclear shielding of the complexes have been studied.

IT 837430-44-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(chiral recognition of model peptides and their fluoro substituted derivs. by DFT calcns.)

RN 837430-44-1 CAPLUS

CN Acetamide, 2,2-difluoro-2-(formylamino)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

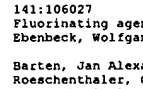
L16 ANSWER 6 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:568191 CAPLUS
DOCUMENT NUMBER: 141:106027
TITLE: Fluorinating agents and process for their preparation
INVENTOR(S): Ebenbeck, Wolfgang; Hilgers, Petra; Marhold, Albrecht;
Barten, Jan Alexander; Kolomeitsev, Alexander; Roeschenthaler, Gerd-Volker
PATENT ASSIGNEE(S): Bayer Chemicals AG, Germany
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1437342	A2	20040714	EP 2003-29976	20031230
EP 1437342	A3	20041006		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10300112	A1	20040715	DE 2003-10300112	20030107
US 2005085474	A1	20050421	US 2004-751623	20040105
JP 2004231646	A2	20040819	JP 2004-1264	20040106
PRIORITY APPLN. INFO.:			DE 2003-10300112 A	20030107

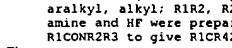
OTHER SOURCE(S): CASREACT 141:106027; MARPAT 141:106027
AB R1CF2NR2R3 [R1 = H, alkyl, alkoxyalkyl, aralkyl, heteroaryl; R2, R3 = aralkyl, alkyl; R1R2, R2R3 = alkylene] and their mixts. with a tertiary amine and HF were prepared for use as fluorinating agents by halogenating R1CONR2R3 to give R1CR42NR2R3 [R4 = Cl, Br] and treating these NaF.
Thus, Me3CONMe2 was converted to Me3CCCl2NMe2 with ClCOCOCl and treated with NaF to give Me2CCF2NMe2. Treatment of HOCHMeCO2Et with Me2CCF2NMe2 gave 81% FCHMeCO2Et.
IT 109797-33-3P 109797-34-4P 721451-42-9P 721451-50-9P 721451-51-0P
RL: IMF (Industrial manufacture); RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorinating agents from amides)
RN 109797-33-3 CAPLUS
CN Ethanamine, N-(difluoromethyl)-N-ethyl- (9CI) (CA INDEX NAME)

RN 109797-34-4 CAPLUS
CN 2-Propanamine, N-(difluoromethyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

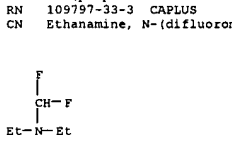
L16 ANSWER 6 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

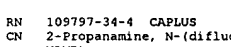


RN 721451-42-9 CAPLUS
CN 1-Propanamine, 1,1-difluoro-N,N,2,2-tetramethyl- (9CI) (CA INDEX NAME)

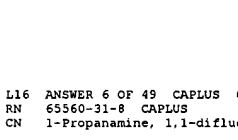


RN 721451-50-9 CAPLUS
CN Ethanamine, N-(difluoromethyl)-N-ethyl-, hydrofluoride (9CI) (CA INDEX NAME)





RN 721451-51-0 CAPLUS
CN 2-Propanamine, N-(difluoromethyl)-N-(1-methylethyl)-, hydrofluoride (9CI) (CA INDEX NAME)



IT 683-81-8P 65560-31-8P 721451-44-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorinating agents from amides)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 6 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 65560-31-8 CAPLUS
CN 1-Propanamine, 1,1-difluoro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)

RN 721451-44-1 CAPLUS
CN 1-Propanamine, N,N-diethyl-1,1-difluoro-2,2-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 7 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:564132 CAPLUS
DOCUMENT NUMBER: 141:125376
TITLE: Manufacture of α,α-difluoramines and difluoromethylene-α,α-diazo compounds as fluorination agents
INVENTOR(S): Ebenbeck, Wolfgang; Marhold, Albrecht; Kolomeitsev, Alexander; Roeschenthaler, Gerd-Volker
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

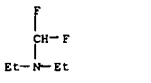
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10300113	A1	20040715	DE 2003-10300113	20030107
EP 1439170	A1	20040721	EP 2003-29973	20031230
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004198975	A1	20041007	US 2004-751824	20040105
US 7045662	B2	20060516		
JP 2004210792	A2	20040729	JP 2004-1699	20040107
PRIORITY APPLN. INFO.:			DE 2003-10300113 A	20030107

OTHER SOURCE(S): CASREACT 141:125376; MARPAT 141:125376
AB R1CF2NR2R3 (R1 = H, C1-12 alkyl, C3-14 aryl, etc.; R2, R3 = C1-12 alkyl, C3-14 aryl, C4-15 aralkyl; R1R2 or R1R3 can form C3-16 carbocyclic ring), agents for fluorination of alcs. and carbonyl compds., especially ketones, carboxylic acids and aldehydes, were prepared with improved yields and without taking special precautionary measures by reacting carbonyl compds. R1CONR2R3 (R1-R2 as above) with (COF)2 or COF2 in a solvent. For example, adding cooled (COF)2 to CH2Cl2 solution of Me3CCONMe2 at -10° in a closed steel reactor and stirring the mixture at room temperature and for 16 h at 40° gave 93% Me3CCF2NMe2 as light yellow liquid
IT 683-81-8 65560-31-8 109797-33-3 721451-44-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination agent; manufacture of α,α-difluoroamines and difluoromethylene-α,α-diazo compds. as fluorination agents)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 65560-31-8 CAPLUS
CN 1-Propanamine, 1,1-difluoro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)

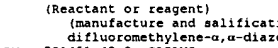
L16 ANSWER 7 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 109797-33-3 CAPLUS
CN Ethanamine, N-(difluoromethyl)-N-ethyl- (9CI) (CA INDEX NAME)

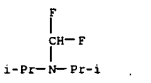


RN 721451-44-1 CAPLUS
CN 1-Propanamine, N,N-diethyl-1,1-difluoro-2,2-dimethyl- (9CI) (CA INDEX NAME)

IT 721451-42-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(manufacture and salification; manufacture of α,α-difluoroamines and difluoromethylene-α,α-diazo compds. as fluorination agents)
RN 721451-42-9 CAPLUS
CN 1-Propanamine, 1,1-difluoro-N,N,2,2-tetramethyl- (9CI) (CA INDEX NAME)



IT 109797-34-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of α,α-difluoroamines and difluoromethylene-α,α-diazo compds. as fluorination agents)
RN 109797-34-4 CAPLUS
CN 2-Propanamine, N-(difluoromethyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

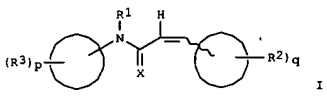


L16 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:370876 CAPLUS
DOCUMENT NUMBER: 140:374987
TITLE: Preparation of aryl and heteroaryl propene amides as antiproliferative agents
INVENTOR(S): Reddy, M. V. Ramana; Reddy, E. Premkumar
PATENT ASSIGNEE(S): Temple University - of the Commonwealth System of Higher Education, USA
SOURCE: PCT Int. Appl., 165 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037751	A2	20040506	WO 2003-US26954	20030828
WO 2004037751	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2497060	AA	20040506	CA 2003-2497060	20030828
AU 2003298567	A1	20040513	AU 2003-298567	20030828
EP 1539675	A2	20050615	EP 2003-796317	20030828
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
NZ 538663	A	20060224	NZ 2003-538663	20030828
JP 2006512306	T2	20060413	JP 2004-546715	20030828
US 2006167317	A1	20060727	US 2005-525553	20050224
PRIORITY APPLN. INFO.:			US 2002-406766P	P 20020829
			WO 2003-US26954	W 20030828

OTHER SOURCE(S): MARPAT 140:374987
GI

L16 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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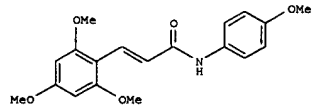
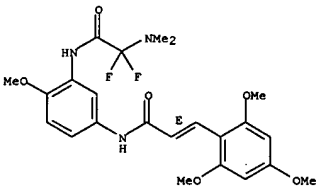


II

AB Title compds. I [A, B = (hetero)aryl; X = O, S; R1 = sulfonylalkyl, acyl, carboxy, etc.; R2 = alkoxy, halo, CN, carboxy, carboxamido, etc.; R3 = halo, alkyl, alkoxy, CN, etc.; p = 1-3; q = 1-5] are prepared For instance,
4-methoxyphenylamino-3-oxopropanoic acid is reacted with 2,4,6-trimethoxybenzaldehyde to give II. Representative examples of activities of compds. I in cell lines (e.g., BT20, DU145) are reported.
I
are useful as antiproliferative agents, radioprotective agents and cytoprotective agents, including, for example, anticancer agents.
IT 684275-95-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl and heteroaryl propene amides as antiproliferative agents)
RN 684275-95-4 CAPLUS
CN 2-Propenamide, N-[3-[[(dimethylamino)difluoroacetyl]amino]-4-methoxyphenyl]-3-(2,4,6-trimethoxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

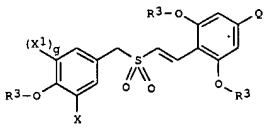
L16 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L16 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:696704 CAPLUS
DOCUMENT NUMBER: 139:230469
TITLE: Preparation of amino-substituted (E)-2,6-dialkoxystyryl 4-substituted benzyl sulfones for treating proliferative disorders
INVENTOR(S): Reddy, Premkumar E.; Reddy, Ramana M. V.; Bell, Stanley C.
PATENT ASSIGNEE(S): Temple University-of the Commonwealth System of Higher Education, USA; Onconova Therapeutics, Inc.
SOURCE: PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072062	A2	20030904	WO 2003-US6357	20030228
WO 2003072062	A3	20031204		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2477232	AA	20030904	CA 2003-2477232	20030228
AU 2003213660	A1	20030909	AU 2003-213660	20030228
EP 1487428	A2	20041222	EP 2003-711347	20030228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005130942	A1	20050616	US 2003-506005	20030228
JP 2005531503	T2	20051020	JP 2003-570809	20030228
PRIORITY APPLN. INFO.:			US 2002-360697P P	20020228
			WO 2003-US6357 W	20030228

OTHER SOURCE(S): MARPAT 139:230469
GI



I

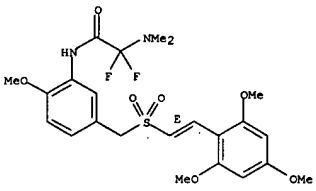
AB Amino-substituted (E)-2,6-dialkoxystyryl 4-substituted benzyl sulfones (shown as I; variables defined below; e.g. (E)-2,4,6-trimethoxystyryl

L16 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
3-(carboxymethylamino)-4-methoxybenzyl sulfone), useful as antiproliferative agents, including, for example, anticancer agents, are provided. The authors believe that I affect the mitogen activated protein kinase (MAPK) signal transduction pathway, thereby affecting tumor cell growth and viability. This cell growth inhibition is assocd. with regulation of the extracellular-signal-regulated kinase (ERK) and c-Jun NH2-terminated kinase (JNK) types of MAPK; I may block the phosphorylating capacity of ERK-2. Tumor cells treated with I are believed to accumulate in the G2/M phase of the cell cycle; as the cells exit the G2/M phase, they appear to undergo apoptosis. Compds. I can readily be covalently bonded to antibodies, preferably tumor-specific monoclonal antibodies (Mab) via a suitable bifunctional linker (-L-) to yield a conjugate I-L-Ab. The effect (IC50 < 10 μM) of .apprx.50 examples of I on prostate carcinoma cell line DU-145, breast adenocarcinoma cell line BT-20, colorectal carcinoma cell line DLD-1 and non-small cell lung carcinoma cell line H157 are tabulated. Fifty-one example prepns. of I are included. For I: X = N(R2)(MyR1), N:CR1R5; X1 = N(R2)(MyR1), N:CR1R5, NO2 (X1 is optionally protected with ≥1 chem. protecting groups); g is 0 or 1; each M is a bivalent connecting group = -(C1-C6)alkylene-, -(CH2)a-V-(CH2)b-, -(CH2)d-W-(CH2)e- and -Z-; each y = 0 and 1; each V = arylene, heteroarylene, -C(O)-, -C(S)-, -S(O)-, -SO2-, -C(O)O-; -C(O)(C1-C6)perfluoroalkylene-, -C(O)NR4-, -C(S)-NR4- and -SO2NR4-; each W = -NR4-, -O- and -S-; a = 0-3; b = 0-3; d = 1-3; e = 0-3. -Z- = -C(O)RaR4N(R4)- wherein the abs. stereochem. of -Z- is D or L or a mixt. of D and L; Ra = -H, -(C1-C6) alkyl, -(CH2)3-NH-C(NH2)(:NH), etc.; R1 = -H, (un)substituted aryl, (un)substituted heterocyclic, -CO2R5, etc.; R2 = -H, -(C1-C6)alkyl, and aryl(C1-C3)alkyl; R3 = -(C1-C6)alkyl; R4 = -H, and-(C1-C6)alkyl; R5 = -H, -(C1-C6)alkyl and -(C1-C6)acyl; R6 = -H, -(C1-C6)alkyl, -CO2R5, -C(O)R7, -OR5, -OC(O)(CH2)2CO2R5, -SR4, guanidino, -NR42, -NR43+, -N+(CH2CH2OR5)3, (un)substituted Ph, (un)substituted heterocyclic and halogen; R7 = -Ra, halogen, -NR42, and heterocycles contg. two N atoms. Q = -H, -(C1-C6)alkoxy, halogen, -(C1-C6)alkyl and -NR42; wherein the substituents for the substituted aryl and substituted heterocyclic groups comprising or included within = halogen, (C1-C6)alkyl, -NO2, -CN, -CO2R5, -C(O)O(C1-C3)alkyl, -OR5, -(C2-C6)-OH, phosphonato, -NR42, - NHC(O)(C1-C6)alkyl, sulfamyl, -OC(O)(C1-C3)alkyl, -O(C2-C6)-N-[(C1-C6)alkyl]2 and -CF3; addnl. details including provisos are given in the claims.

IT 592543-18-5P, (E)-2,4,6-Trimethoxystyryl 3-(2-dimethylamino-2,2-difluoroacetamido)-4-methoxybenzyl sulfone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of amino-substituted (E)-2,6-dialkoxystyryl 4-substituted benzyl sulfones for treating proliferative disorders)
RN 592543-18-5 CAPLUS
CN Acetamide, 2-(dimethylamino)-2,2-difluoro-N-[2-methoxy-5-[[[(1E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L16 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 592543-19-6, α-Dimethylamino-α,α-difluoroacetyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amino-substituted (E)-2,6-dialkoxystyryl 4-substituted benzyl sulfones for treating proliferative disorders)
RN 592543-19-6 CAPLUS
CN Acetyl chloride, (dimethylamino)difluoro- (9CI) (CA INDEX NAME)

L16 ANSWER 10 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:666318 CAPLUS
DOCUMENT NUMBER: 138:72869
TITLE: A theoretical analysis of substituted formamide conformers
AUTHOR(S): Headley, Allan D.; Nam, Jaewook
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409-1061, USA
SOURCE: THEOCHEM (2002), 589-590, 423-429
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Twelve conformers of substituted formamides, X-NHC(O)H, where X represents CH3, CH2F, CHF2 and CF3 were examined by ab initio calcns. The relatively small dipole moment of cis N-trifluoromethyl formamide (1.4 D) contributes to it being more stable than the trans conformer (4.8 D). The energy difference between these two conformers, calculated at the MP2/6-31+G* level of theory, is 1.4 kcal/mol. On the other hand, even though the cis and trans conformers of N-Me formamide have similar dipole moments (4.8 and 4.5 D, resp.), the trans conformer is more stable than the cis conformer by 1.4 kcal/mol. A difference in dipole moments may not be the only factor to account for this energy difference. Since the distance between the carbonyl oxygen and the N-Me substituent of trans N-Me formamide is shorter than expected, a possible interaction exists between these two groups. Such an interaction would contribute to the unexpected stability of trans N-Me formamide. For trans N-trifluoromethyl formamide, a similar type interaction between these two groups does not exist and the difference in dipole moment is the dominant factor that dets. the most stable conformer. The results of a similar anal. of fluoromethyl formamide and difluoromethyl formamide are also discussed.

IT 481072-18-8
RL: PRP (Properties)
(ab initio study on conformational stability of substituted formamide)
RN 481072-18-8 CAPLUS
CN Formamide, N-(difluoromethyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:309498 CAPLUS
DOCUMENT NUMBER: 131:73199
TITLE: Carbenoid reactions of trifluoromethyl element compounds. Part 5. Difluoromethylation of amines with Zn(CF3)Br.2MeCN, Cd(CF3)2.2MeCN, and the system Bi(CF3)3/AlCl3
AUTHOR(S): Pasenok, S. V.; Kirij, N. V.; Yagupolskii, Yu. L.; Naumann, Dieter; Tyrra, W.; Fitzner, A.
CORPORATE SOURCE: Institute Organic Chemistry, Natl. Acad. Sci. Ukraine, Kiev, Ukraine
SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1999), 625(5), 834-838
CODEN: ZAACAB; ISSN: 0044-2313
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:73199

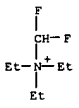
AB The reactions of Zn(CF3)Br.2MeCN, Cd(CF3)2.2MeCN, or Bi(CF3)3/AlCl3 with tertiary amines lead to the formation of quaternary ammonium salts of the general formula [R3NCHF2]X. The reaction of 4-(dimethylamino)pyridine with Zn(CF3)Br.2MeCN yields 4-[(difluoromethyl)dimethylamino]pyridinium bromide. Bi(CF3)3/AlCl3 reacts with 1,4-diazabicyclo[2.2.2]octane to form a mixture of mono- and bis[(difluoromethyl)ammonium] salts.

IT 229183-31-7P
RL: BYP (Byproduct); PREP (Preparation)
(difluoromethylation with (trifluoromethyl)zinc bromide and (trifluoromethyl)cadmium acetonitrile complexes, or (trifluoromethyl)bismuth)

RN 229183-31-7 CAPLUS
CN Ethanaminium, N-(difluoromethyl)-N,N-diethyl-, (T-4)-tetrafluoroaluminate(1-) (9CI) (CA INDEX NAME)

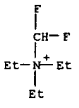
CM 1

CRN 124462-77-7
CMF C7 H16 F2 N

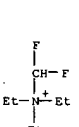


CM 2

CRN 21340-02-3
CMF Al F4
CCI CCS



L16 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● Br⁻

RN 229183-27-1 CAPLUS
CN Ethanaminium, N-(difluoromethyl)-N,N-diethyl-, (T-4)-tetrachlorobismuthate(1-) (9CI) (CA INDEX NAME)

CM 1

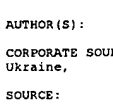
CRN 124462-77-7
CMF C7 H16 F2 N

CM 2

CRN 20057-70-9
CMF Bi Cl4
CCI CCS

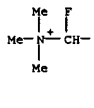
REFERENCE COUNT: 19 THIS FORMAT
THERE ARE 19 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

L16 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



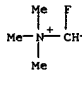
IT 98181-98-7P 229183-25-9P 229183-26-0P
229183-27-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(difluoromethylation with (trifluoromethyl)zinc bromide and (trifluoromethyl)cadmium acetonitrile complexes, or (trifluoromethyl)bismuth)

RN 98181-98-7 CAPLUS
CN Methanaminium, 1,1-difluoro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

RN 229183-25-9 CAPLUS
CN Methanaminium, 1,1-difluoro-N,N,N-trimethyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 229183-26-0 CAPLUS
CN Ethanaminium, N-(difluoromethyl)-N,N-diethyl-, bromide (9CI) (CA INDEX NAME)

L16 ANSWER 12 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:803739 CAPLUS
DOCUMENT NUMBER: 128:28030
TITLE: Conformable nickel coating and process for coating an article with a conformable nickel coating
INVENTOR(S): Abys, Joseph Anthony; Kadija, Igor Veljko; Fan, Chonglun
PATENT ASSIGNEE(S): Lucent Technologies Inc., USA
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 811706	A1	19971210	EP 1997-303564	19970527
EP 811706	B1	20010620		
R: DE, GB				
US 5916696	A	19990629	US 1996-660628	19960606
JP 10060685	A2	19980303	JP 1997-149114	19970606
JP 3266545	B2	20020318		
HK 1004817	A1	20010928	HK 1998-103990	19980508
PRIORITY APPLN. INFO.:			US 1996-660628 A	19960606

AB The present invention is directed to a lead frame in which the metal lead frame substrate is copper, copper alloy, or nickel alloy. The lead frame substrate is coated with a conformable nickel coating that is crack-resistant when the lead frame is bent to an angle of at least 82° with a bend radius of about 150 μm to about 300 μm. Bending the lead frame in this manner causes surface deformations in the lead frame substrate. Cracks do not appear through the thickness of the conformable nickel coating of the present invention when the depth of the deformations that result from this bending do not exceed about 5 μm.

IT 199483-47-1, Perfluorododecyltrimethylammonium fluoride
RL: MOA (Modifier or additive use); USES (Uses)
(electroplating of conformable nickel on metal lead frames from bath containing)

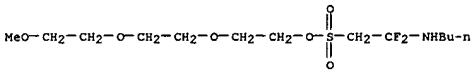
RN 199483-47-1 CAPLUS
CN 1-Dodecanaminium, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-pentacosafluoro-N,N,N-trimethyl-, fluoride (9CI) (CA INDEX NAME)

● F⁻

L16 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:609476 CAPLUS
DOCUMENT NUMBER: 123:280274
TITLE: Modification and immobilization of proteins with polyethylene glycol tresylates and polysaccharide tresylates: evidence suggesting a revision of the coupling mechanism and the structure of the polymer-polymer linkage
AUTHOR(S): Gais, Hans-Joachim; Ruppert, Stephan
CORPORATE SOURCE: Inst. Org. Chem., RWTH Aachen, Aachen, 52056, Germany
SOURCE: Tetrahedron Letters (1995), 36(22), 3837-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The isolation of sulfonate-amide from the reaction of tresylate with butylamine in aqueous buffer solution at pH 8.0 suggests a new mechanism for the modification and immobilization of proteins with polyethylene glycol monomethyl ether tresylate and polysaccharide tresylates.

IT 169311-34-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(modification and immobilization of proteins with polyethylene glycol tresylates and polysaccharide tresylates: evidence suggesting a revision of the coupling mechanism and the structure of the polymer-polymer linkage)
RN 169311-34-6 CAPLUS
CN Ethanesulfonic acid, 2-(butylamino)-2,2-difluoro-, 2-[2-(2-methoxyethoxy)ethoxy]ethyl ester (9CI) (CA INDEX NAME)



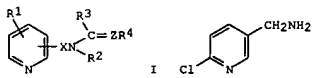
L16 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:492085 CAPLUS
DOCUMENT NUMBER: 115:92085
TITLE: Preparation of pyridylalkylamine derivatives as insecticides
INVENTOR(S): Ishimitsu, Keiichi; Suzuki, Junji; Ohishi, Haruhito; Yamada, Tomio; Hatano, Renpei; Takakusa, Nobuo; Mitsui, Jun
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9104965	A1	19910418	WO 1990-JP1282	19901004
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CM, DE, DK, ES, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
ZA 9007775	A	19910731	ZA 1990-7775	19900928
CA 2041670	AA	19910407	CA 1990-2041670	19901004
CA 2041670	C	19970318		
AU 9065117	A1	19910428	AU 1990-65117	19901004
AU 633991	B2	19930211		
EP 456826	A1	19911121	EP 1990-914758	19901004
EP 456826	B1	19990107		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
HU 57191	A2	19911128	HU 1990-7896	19901004
HU 214992	B	19981228		
BR 9006961	A	19911217	BR 1990-6961	19901004
JP 04154741	A2	19920527	JP 1990-264968	19901004
JP 2926954	B2	19990728		
RO 112865	B1	19980130	RO 1990-147641	19901004
AT 175405	E	19990115	AT 1990-914758	19901004
ES 2127718	T3	19990501	ES 1990-914758	19901004
HU 220083	B	20011028	HU 1998-2249	19901004
CN 1050714	A	19910417	CN 1990-108265	19901006
CN 1056958	B	20001004		
IL 98014	A1	19960804	IL 1991-98014	19910501
RU 2038352	C1	19950627	RU 1991-4895590	19910605
US 5304566	A	19940419	US 1991-700165	19910709
LV 10155	B	19950820	LV 1992-617	19921230
LT 3209	B	19950327	LT 1993-342	19930213
US 5612358	A	19970318	US 1993-117470	19930907

PRIORITY APPLN. INFO.:

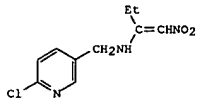
JP 1989-259966	A	19891006
JP 1989-336231	A	19891227
JP 1990-56611	A	19900309
JP 1990-115246	A	19900502
JP 1990-196258	A	19900726
WO 1990-JP1282	A	19901004
US 1991-700165	A1	19910709

L16 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 115:92085
GI



I

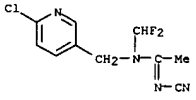
II



III

AB The title compds. [I; R1 = H; substituent; R2 = H, (substituted) (thio)carbamoyl, sulfamoyl, (substituted) C1-5 alkyl, C2-5 alkenyl, alkynyl etc.; R3 = H, (substituted) C1-5 alkyl, C2-5 alkenyl, alkynyl, C3-8 cycloalkyl, etc., R4 = cyano, NO2; X = (substituted) C1-3 alkylene, alkylidene; Z = CH, N] or their salts are prepared A mixture of amine II 4.2, EtCOCH2NO2 3.5, and p-MeC6H4SO3H 0.1 g in MePh was refluxed to give 4.1 g III, which killed 100% cotton aphids and green rice leafhopper at 125 ppm. Also prepared and tested were 111 addnl. I.

IT 135410-38-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as insecticide)
RN 135410-38-7 CAPLUS
CN Ethanimidamide, N-[(6-chloro-3-pyridinyl)methyl]-N'-cyano-N-(difluoromethyl)- (9CI) (CA INDEX NAME)

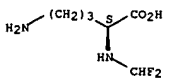


L16 ANSWER 15 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:210653 CAPLUS
DOCUMENT NUMBER: 112:210653
TITLE: Inhibition of transformation in cultured rat tracheal epithelial cells by potential chemopreventive agents
AUTHOR(S): Steele, Vernon E.; Kelloff, Gary J.; Wilkinson, Betty P.; Arnold, Julia T.
CORPORATE SOURCE: Environ. Sci. Div., NSI Technol. Serv. Corp., Research Triangle Park, NC, 27709, USA
SOURCE: Cancer Research (1990), 50(7), 2068-74
CODEN: CNREA8; ISSN: 0008-5472
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A group of 28 compds. was screened for chemopreventive activity in a rat tracheal epithelial cell transformation inhibition assay. The chems. were tested for their ability to inhibit the formation of transformed rat tracheal epithelial cell colonies which arise following exposure to the carcinogen benzo[a]pyrene. The 15 active compds. were N-acetylcysteine, bismuththiol, Ca glucarate, (±)-catechin, diallyl disulfide, glycaric acid, D-glucaro-1,4-lactone, N-(4-hydroxyphenyl)retinamide, d-limonene, mesna, retinoic acid, rutin, quercetin, silymarin, and taurine. Several possible chemopreventive mechanisms appeared to be predominant. The active compds. increased glutathione levels or enhanced conjugation, increased cytochrome P 450 activity, displayed nucleophilic activity, or induced differentiation. The remaining 13 compds. were neg. in the assay: crocetin, difluoromethylorinithine, ellagic acid, esculetin, enoxolone, ibuprofen, levamisole, nordihydorguaiaretic acid, L-2-oxothiazolidine-4-carboxylate, piroxicam, sodium butyrate, d-α-tocopherol acetate, and polyethylene glycol 400. This assay could not detect compds. that were antipromoting in nature, glutathione inhibitors, differentiation inhibitors, O6-methylguanine inhibitors, organ specific, or inactive. The assay appeared to identify chemopreventive compds. that act at early stages of the carcinogenic process.

IT 102786-93-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of, cell transformation assay for)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

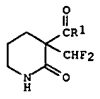
Absolute stereochemistry.



L16 ANSWER 16 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:178093 CAPLUS
DOCUMENT NUMBER: 112:178093
TITLE: Preparation of dialkyl 2-difluoromethyl-2-(2-cyanoethyl)malonates and their use in synthesis of D,L-α-(difluoromethyl)ornithine
INVENTOR(S): Mettler, Hanspeter; Greth, Erich
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Patentschrift (Switz.), 5 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 672124	A	19891031	CH 1987-2539	19870703
PRIORITY APPLN. INFO.:			CH 1987-2539	19870703

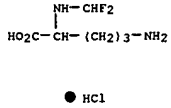
OTHER SOURCE(S): CASREACT 112:178093; MARPAT 112:178093
GI



III

AB F2CHC(CO2R)2CH2CH2CN (I; R = Me, Et) were prepared and used as precursors for the synthesis of difluoromethylornithine (II), less expensive than the currently used ornithine. CH2(CO2Me)2 underwent successive alkylations with CH2:CHCN and CH2F2 to give I (R = Me) which was cyclized to piperidone III (R1 = MeO) by hydrogenation. This was amidated with NH3 and the amide (III; R1 = NH2) reacted with hypochlorite and alkali to give the title ornithine derivative Alternatively III (R1 = Et) underwent an ester hydrazinolysis and the resulting hydrazide (III; R1 = NHNH2) was converted to the title ornithine via the corresponding azide and isocyanate.
IT 126309-12-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 126309-12-4 CAPLUS
CN Ornithine, N2-(difluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L16 ANSWER 16 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

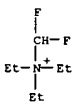


● HCl

L16 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:118217 CAPLUS
DOCUMENT NUMBER: 112:118217
TITLE: Inverse amine-stabilized sulfenes F2C:SO2 and FHC:SO2
AUTHOR(S): Pritzkow, Hans; Rall, Klaus; Reimann-Andersen, Stefan; Sundermeyer, Wolfgang
CORPORATE SOURCE: Anorg. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900/1, Germany
SOURCE: Angewandte Chemie (1990), 102(1), 80-1
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 112:118217
AB Et3N+CRFSO2- (I, R = H) was obtained by treatment of FCH2SO2Cl with Et3N in THF, and I (R = F) was obtained by similar treatment of tetrafluoro-1,3-dithietane 1,1,3,3-tetroxide. X-ray anal. of I (R = H, F) demonstrated the zwitterionic character of these species.
IT 124462-78-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124462-78-8 CAPLUS
CN Ethanaminium, N-(difluoromethyl)-N,N-diethyl-, sulfite (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 124462-77-7
CMF C7 H16 F2 N

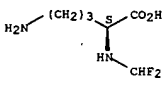


CM 2

CRN 15181-46-1
CMF H O3 S

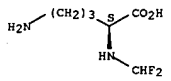
L16 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:69566 CAPLUS
DOCUMENT NUMBER: 112:69566
TITLE: Chemosensitization, chromatin condensation, and cell cycle related effects of difluoromethylornithine-induced polyamine depletion in human adenocarcinoma cells
AUTHOR(S): Block, Adrienne Lee
CORPORATE SOURCE: Northwestern Univ., Evanston, IL, USA
SOURCE: (1989) 302 pp. Avail.: Univ. Microfilms Int., Order No. DA8913956
From: Diss. Abstr. Int. B 1989, 50(4), 1337
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 102786-93-6
RL: BIOL (Biological study)
(polyamine depletion induced by, in human adenocarcinoma, antitumor drug mechanism in relation to)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



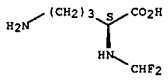
L16 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:608830 CAPLUS
DOCUMENT NUMBER: 111:208830
TITLE: Chemoprevention of mouse colon tumors with difluoromethylornithine during and after carcinogen treatment
AUTHOR(S): Tempero, Margaret A.; Nishioka, Kenji; Knott, Kristen;
Zetterman, Rowan K.
CORPORATE SOURCE: Omaha Veterans Adm. Med. Cent., Omaha, NE, 68105, USA
SOURCE: Cancer Research (1989), 49(21), 5793-7
CODEN: CNREA8; ISSN: 0008-5472
DOCUMENT TYPE: Journal
LANGUAGE: English
AB α-Difluoromethylornithine (DFMO) treatment has been shown to modify carcinogenesis in many exptl. tumor models, including skin, breast, and colon. This study was designed to determine whether DFMO treatment can inhibit exptl. mouse colon tumors after carcinogen treatment and whether an associated effect of DFMO on cell proliferation in colon mucosa occurs. Male CD1 mice received dimethylhydrazine and various schedules of DFMO, 1% in drinking water; Group A, none; Group B, following dimethylhydrazine treatment; Group C, during dimethylhydrazine treatment; and Group D, continuously throughout the study. Measurements of erythrocyte polyamine levels showed that DFMO treatment ablated putrescine levels and confirmed that a systemic biol. effect was achieved. Anal. of tumor data showed a significant inhibitory effect of DFMO treatment on colon tumor (adenomas and adenocarcinomas) incidence in Groups B (24%) and D (20%) compared to control Group A and on squamous cell carcinomas of the anus in all groups. No consistent effect of DFMO treatment on cell proliferation in colon mucosa was identified. This study supports the hypothesis that DFMO treatment alters events in the postinitiation phases of mouse colon tumorigenesis.
IT 102786-93-6
RL: BIOL (Biological study)
(colon neoplasm inhibition by, after induction with dimethylhydrazine)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



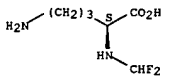
L16 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:590382 CAPLUS
DOCUMENT NUMBER: 111:190382
TITLE: Epidermal photosensitization by psoralens: protective effect of vitamins A and E on polyamine and free radical metabolism
AUTHOR(S): Khettab, N.; Amory, M. C.; Briand, G.; Bousquet, B.; Forlot, P.; Barey, M.; Combre, A.
CORPORATE SOURCE: Lab. Biochim. Physiol., Fac. Pharm., Nantes, 44025, Fr.
SOURCE: Psoralens, Proc. Int. Congr. "Psoralens 1988" (1989), Meeting Date 1988, 207-12. Editor(s): Fitzpatrick, Thomas B. Libbey: Paris, Fr.
CODEN: 56PZAJ
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The photoprotective effect of vitamins A and E in skin due to inhibition of polyamine synthesis and production of free radicals was confirmed. These variables were measured in the lumbar epidermis of the female hairless mouse subjected to UV A + B irradiation Polyamines were assayed in epidermal homogenate by HPLC, and production of oxygenated free radicals was determined by spectrofluorometric assay of malonyldialdehyde. Butylhydroxytoluene and vitamin E inhibited production of oxygenated free radicals and epidermal biosynthesis of polyamines, whereas the inhibitory effect of malonyldialdehyde induced by vitamin A had no associated effect on polyamine metabolism
IT 102786-93-6
RL: BIOL (Biological study)
(photoprotection by, of skin epidermis from psoralen photosensitization, polyamine metabolism and radicals in relation to)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



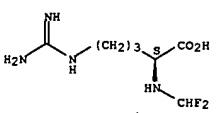
L16 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:420764 CAPLUS
DOCUMENT NUMBER: 111:20764
TITLE: In vitro effect of polyamine biosynthesis inhibitors on Toxoplasma gondii
AUTHOR(S): Derouin, F.
CORPORATE SOURCE: Lab. Parasitol.-Mycol., Hop. St.-Louis, Paris, 75010, Fr.
SOURCE: Bulletin de la Societe Francaise de Parasitologie (1988), 6(1), 33-9
CODEN: BSFPE9; ISSN: 0761-8328
DOCUMENT TYPE: Journal
LANGUAGE: French
AB The effect of 4 polyamine biosynthesis inhibitors was evaluated in vitro using an enzyme immunoassay performed directly on the infected cultures. A significant inhibitory effect was observed with the ornithine decarboxylase inhibitors for concns. of 10-50 mM for difluoromethylornithine, 1-5 mM for methylacetylenic putrescine, and 0.4-8 mM for monofluoromethyldehydroornithine Me ester. Only a partial inhibitory effect was noted with difluoromethylarginine, an arginine decarboxylase inhibitor, at concentration close to those that gave nonspecific toxicity on the monolayers.
IT 102786-93-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Toxoplasma gondii response to)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



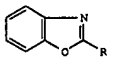
L16 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:404648 CAPLUS
DOCUMENT NUMBER: 111:4648
TITLE: Peptide analogs of the mud crab pumping pheromone: structure-function studies
AUTHOR(S): Rittschof, D.; Forward, R. B., Jr.; Simons, Delora A.;
Reddy, P. Amantha; Erickson, Bruce W.
CORPORATE SOURCE: Mar. Lab., Duke Univ., Beaufort, NC, 28516, USA
SOURCE: Chemical Senses (1989), 14(1), 137-48
CODEN: CHSED8; ISSN: 0379-864X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the mud crab, Rhithropanopeus harrisii, larval release is highly synchronous and is controlled by peptide pheromones released from the hatching eggs. The pheromones and synthetic peptide analogs, containing neutral amino acids as the amino-terminus and a basic amino acid at the carboxy-terminus, evoke larval release of pumping behavior in the female. Structure-function relationships between behavioral responses and peptide analogs of the pumping pheromone are described. Compds. tested included 11 peptides containing 1-7 neutral amino acid residues and a carboxy-terminal arginine residue, and modified arginine compds. Complex feeding stimulant mixts. and groups of peptides were tested to provide information about the number of different types of receptors. Pumping behavior was described in terms of response threshold, maximum percentage response, and effective concentration range. All carboxy-terminal arginine peptides tested evoked pumping responses. Response thresholds ranged from 10-15M for the most potent peptide Ile-Gly-Arg to 10-8M for the least potent Tyr-Arg. Effective concentration ranges for the peptides varied from one to four orders of magnitude and the responses normally declined with further increase in concentration Maximum percentage response was largely independent of response threshold and ranged from 30-60%, comparable to assay responses of larval hatch water. Responses within size groups of peptides were more similar than between groups. Studies with modified arginines showed that hydrophobic structures similar in size and shape to small peptides evoked responses. Sterically hindered hydrophobic moieties were ineffective. Tests with mixts. of active compds. support the hypothesis that there is one type of pumping peptide receptor.
IT 121038-35-5
RL: BIOL (Biological study)
(larva response to, in mud crab, structure in relation to)
RN 121038-35-5 CAPLUS
CN L-Arginine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

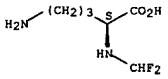
L16 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:57553 CAPLUS
DOCUMENT NUMBER: 110:57553
TITLE: Synthesis of 2-(dichloromethyl)- and 2-(difluoromethyl)benzoxazoles
AUTHOR(S): Liska, Frantisek; Vagner, Josef; Dedek, Vaclav
CORPORATE SOURCE: Dep. Org. Chem., Vys. Sk. Chemickotechnol., Prague, Czech.
SOURCE: Sbornik Vysoke Skoly Chemicko-Technologicke v Praze, C: Organicka Chemie a Technologie (1986), C29, 37-43
CODEN: SVOCAF; ISSN: 0554-9728
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:57553
GI



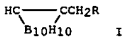
AB Benzoxazoles I (R = CHCl2, CHFCl) were prepared by the cyclocondensation of 2-aminophenol with RCF2NEt2. I (R = CHFCl) reacted with KF in DMF to give I (R = CHF2).
IT 67406-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of, with aminophenol, benzoxazole derivative from)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)

L16 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:485881 CAPLUS
DOCUMENT NUMBER: 109:85881
TITLE: Polyamines increase in human peripheral blood and bone marrow mononuclear cells following administration of methylglyoxal bis(guanylhydrazone)
AUTHOR(S): Maddox, Anne Marie; Keating, Michael J.; Freireich, Emil J.; Haddox, Mari K.
CORPORATE SOURCE: Med. Sch., Univ. Texas, Houston, TX, 77030, USA
SOURCE: Chemotherapy (Basel, Switzerland) (1988), 34(5), 419-29
CODEN: CHTHBK; ISSN: 0009-3157
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Eight patients who had refractory leukemia and 1 patient with refractory multiple myeloma were treated with the polyamine biosynthesis inhibitors methylgloxal bis(guanylhydrazone) (MGBG) and difluoromethylornithine (DFMO). After the first dose of MGBG there was an increase in polyamine content in the mononuclear cells of both the peripheral blood and the bone marrow despite the administration of DFMO in all patients with leukemia. Putrescine levels increased in the mononuclear cells of all patients, cellular spermidine levels increased in 4 and cellular spermine levels increased in 5 patients. The cellular polyamine levels remained elevated above the pretreatment levels for up to 1 wk in some patients. Subsequent treatment with MGBG, administered after 1-2 wk of DFMO treatment, also promoted increases in mononuclear cell polyamine concns. Since enhanced tumor cell uptake of MGBG after DFMO priming is hypothesized to be dependent on a decrease in cellular polyamine levels, the increase in cellular polyamines after MGBG has important implications for the scheduling of this drug combination. From these observations, withholding MGBG until DFMO treatment has produced a decrease in tumor cell polyamine concns. would be the schedule most likely to enhance the uptake of MGBG.
IT 102786-93-6
RL: BIOL (Biological study)
(leukemia and myeloma treatment with methylglyoxalbis(guanylhydrazone) and, polyamine formation increase in mononuclear leukocytes in, in humans)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:204662 CAPLUS
DOCUMENT NUMBER: 108:204662
TITLE: Alkylation of aromatic hydrocarbons by 1-(fluoromethyl)-o,m-carboranes and aluminum chloride
AUTHOR(S): Lebedev, V. N.; Balagurova, E. V.; Zakharkin, L. I.
CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1987), (5), 1134-6
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 108:204662
GI



AB The title carboranes undergo Friedel-Crafts reactions with aromatic hydrocarbons. Thus, treating carborane I (R = F) with C6H6, MePh, and p-MeC6H4Me in the presence of AlCl3 gave I (R = Ph, C6H4Me, C6H3Me2).
IT 683-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (hydroxymethyl)carborane)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

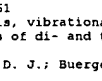
L16 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:477261 CAPLUS
DOCUMENT NUMBER: 107:77261
TITLE: Synthesis, vibrational spectra, and crystal structure analysis of di- and trifluoro-tetramethylammonium salts
AUTHOR(S): Brauer, D. J.; Buerger, H.; Grunwald, M.; Pawelke, G.; Wilke, J.
CORPORATE SOURCE: Anorg. Chem., Univ. Gesamthochsch., Wuppertal, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1986), 537, 63-78
CODEN: ZAACAB; ISSN: 0044-2313
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 107:77261
AB Tetramethylammonium salts, Me3 N+CH2F (I), Me3N+CHF2 (II), and Me3N+CF3 (III), were prepared by quaternization of the corresponding fluoromethylamines. II was also generated from Me3N and Zn-CF2Br2-KF in MeCN. I, II, and III were characterized by NMR and vibrational spectroscopy, a normal coordinate anal. being undertaken for III. The crystal structures of the iodides of II and III have been determined In both cations the N-Me distances are on the average (II 1.508(2) Å; III 1.514(5) Å) longer than the N-CF valencies (II 1.497(4) Å; III 1.491(6) Å).
IT 109797-39-9P 109797-40-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 109797-39-9 CAPLUS
CN Ethanaminium, N-(difluoromethyl)-N-ethyl-N-methyl-, iodide (9CI) (CA INDEX NAME)

● I⁻

RN 109797-40-2 CAPLUS
CN Benzenaminium, N-(difluoromethyl)-N,N-dimethyl-, iodide (9CI) (CA INDEX NAME)

L16 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L16 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● I⁻

IT 109797-37-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, NMR, and crystal structure of)
RN 109797-37-7 CAPLUS
CN Methanaminium, 1,1-difluoro-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)

● I⁻

IT 683-81-8P 109797-33-3P 109797-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, NMR, and quaternization of, with Me iodide)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 109797-33-3 CAPLUS
CN Ethanamine, N-(difluoromethyl)-N-ethyl- (9CI) (CA INDEX NAME)

RN 109797-34-4 CAPLUS
CN 2-Propanamine, N-(difluoromethyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

L16 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:487395 CAPLUS
DOCUMENT NUMBER: 105:87395
TITLE: Electrochemical fluorination of chlorofluoroalkylamines
AUTHOR(S): Hayashi, Eiji; Abe, Takashi; Baba, Hajime; Nagase, Shunji
CORPORATE SOURCE: Gov. Ind. Res. Inst., Nagoya, 462, Japan
SOURCE: Nagoya Kogyo Gijutsu Shikensho Hokoku (1985), 34(4/5), 117-22
CODEN: NKGSAR; ISSN: 0027-7614
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Electrolytic fluorination of chlorofluoroalkylamine derivs. (I) was effected by electrolyzing 20 g I in 500 mL HF at an anodic c.d. of 3.3 A/dm2 and 6.6-7 V at 5-12° for 220 min. Thus, N-(2,2-dichloro-1,1-difluoroethyl)piperidine yielded dichloroperfluoro-, chloroperfluoro- and perfluoro-derivs. in 0.8-1.4, 7.1-8.7 and 27.6-33%, resp., while N-(2,2-dichloro-1,1-difluoroethyl)-morpholine and -pyrrolidine, N-(2-chloro-2-fluoro-1,1-difluoroethyl)piperidine, N-(2,2-dichloro-1,1-difluoroethyl)-dipropyl- and dibutyl-amines yielded perfluoro- and chloroperfluoro-derivs. in 13.5-27 and 4.5-7.7%, resp., and N-(2-chloro-2-fluoro-1,1-difluoroethyl)- and N-(2,2-dichloro-1,1-difluoroethyl)-diethylamines yielded perfluoro-, hydroperfluoro, chloroperfluoro- and chloro-hydro-perfluoro-derivs. in 24.1-36, 2.5-3.5, 11.5-14.9 and 0.2-0.9% yields, resp.
IT 67406-60-4 103811-93-4 103811-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of, electrochem.)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)

RN 103811-93-4 CAPLUS
CN 1-Propanamine, N-(2,2-dichloro-1,1-difluoroethyl)-N-propyl- (9CI) (CA INDEX NAME)

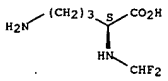
RN 103811-94-5 CAPLUS
CN 1-Butanamine, N-butyl-N-(2,2-dichloro-1,1-difluoroethyl)- (9CI) (CA INDEX NAME)

L16 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:417927 CAPLUS
DOCUMENT NUMBER: 105:17927
TITLE: Combined effects of α-difluoromethylornithine and doxorubicin against pancreatic cancer cell lines in culture
AUTHOR(S): Chang, Barbara K.; Gutman, Robert; Black, Owen, Jr.
CORPORATE SOURCE: Dep. Med., Med. Coll. Georgia, Augusta, GA, USA
SOURCE: Pancreas (1986), 1(1), 49-54
CODEN: PANCE4; ISSN: 0885-3177
DOCUMENT TYPE: Journal
LANGUAGE: English

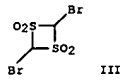
AB Pancreatic adenocarcinoma presents a clin. and exptl. challenge because of its relative resistance to conventional modes of therapy. A novel, biol. based approach to enhancing its chemosensitivity and to overcoming its chemoresistance in a panel of pancreatic adenocarcinoma cell lines (two human lines: PANC-1 and COLO-357; and two hamster lines: WD PaCa and PD PaCa) was studied. Difluoromethylornithine (DFMO) [102786-93-6], a specific inhibitor of ornithine decarboxylase (ODC) [9024-60-6] that produces antiproliferative effects by polyamine depletion, was combined with the cytotoxic agent doxorubicin (DOX) [23214-92-8] in vitro. The inhibitory effects of DFMO were cytostatic and roughly additive to those of DOX. Although the response to the combination varied as a function of the cell lines studied and the response to DFMO as a single agent, all cell lines studied showed some increased inhibition with the combination. The most striking enhancement was seen in the most DOX-resistant cell line, WD PaCa, and also in PAN-1, a relatively sensitive cell line. Thus, the combination of DFMO and DOX shows promise as an exptl. approach to the problem of drug resistance and the limited chemosensitivity of pancreatic cancer.

IT 102786-93-6
RL: BIOL (Biological study)
(neoplasm inhibition by doxorubicin combined with, against adenocarcinoma cell lines of humans and laboratory animals)
RN 102786-93-6 CAPLUS
CN L-Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



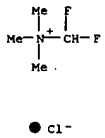
L16 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:522952 CAPLUS
DOCUMENT NUMBER: 103:122952
TITLE: Reactions of halogenated methanesulfonyl chlorides with trimethylamine and an inverse sulfene-amine adduct.
AUTHOR(S): Rheude, Udo; Sundermeyer, Wolfgang
CORPORATE SOURCE: Anorg.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900/1, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1985), 118(6), 2208-19
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 103:122952
GI



III

AB BrCH2Cl reacted with KF to give FCH2Cl which reacted with, e.g., Ph2CHSH to give Ph2CHSCH2SH. This was oxidized with Cl-H2O to give FCH2SO2Cl (I). I formed the adduct Me3N+CHFSO2- with Me3N. BrCH2SO2Cl gave mainly BrCH2SO2C-RSO2N+Me3 (II, R = H), along with some II (R = Br). Several other reactions were studied; e.g., the dithietane III was prepared

IT 98181-98-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 98181-98-7 CAPLUS
CN Methanaminium, 1,1-difluoro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

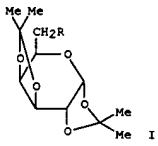


L16 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:78293 CAPLUS
DOCUMENT NUMBER: 102:78293
TITLE: Synthesis and reactions of fluorinated iminium salts
AUTHOR(S): Henle, H.; Geisel, M.; Mews, R.
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Goettingen, Goettingen, D-3400, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1984), 26(2), 133-48
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 102:78293

AB [RR1C:NR2R3]+ MF6- (R = R1 = F, R2 = R3 = Me, Et, M = As, Sb; R = H, R1 = F, R2 = R3 = Me, M = As, Sb; R = R1 = CF3, R2 = H, R3 = Me, M = Sb; R = R1 = CF3, R2 = R3 = Me, M = As) were prepared either by alkylations with MeOSO+ MF6- or by F- abstraction with MF5 (M = As, Sb). IR spectra and NMR of these salts were briefly discussed. Dialkyl(perfluoroalkyl)amines, e.g. (F3C)2CFNMe2, were prepared by F- addition to the title salts. Methylating F3CN:CF2 gave (F3C)2NMe.

IT 683-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with arsenic or antimony pentafluoride)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

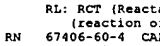
L16 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:139492 CAPLUS
DOCUMENT NUMBER: 100:139492
TITLE: Reaction behavior of chlorofluorotriethylamines with galactose
AUTHOR(S): Zeisig, Reinhardt; Cech, Dieter; Liska, Frantisek; Dedek, Vaclav
CORPORATE SOURCE: Sekt. Chem., Humboldt-Univ. Berlin, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1983), 23(10), 375
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

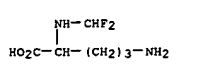
AB Treating galactopyranose I (R = OH) with ClFCHCF2NEt2 or Cl2CHCF2NEt2 in DMF gave 24.3 and 19.3% I (R = Cl), resp., in addition to I (R = O2CCHFCl) and 51% I (R = O2CCHCl2).

IT 67406-60-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diisopropylidenegalactopyranose)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)



L16 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:51044 CAPLUS
DOCUMENT NUMBER: 100:51044
TITLE: Reaction of tertiary formamides with sulfur tetrafluoride. Direct synthesis of (trifluoromethyl)amines
AUTHOR(S): Dmowski, Wojciech; Kaminski, Maciej
CORPORATE SOURCE: Inst. Org. Chem., Pol. Acad. Sci., Warsaw, 00-961, Pol.
SOURCE: Journal of Fluorine Chemistry (1983), 23(3), 207-18
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:51044
AB Treating RR1NCHO (R = R1 = Me, Et; R = Ph, R1 = Et; NRR1 = morpholino, piperidino) with SF4 in the presence of KF directly converted CHO to CF3 to give 89-94% RR1NCF3. Hydrolysis of RR1NCF3 (R = R1 = Me, Et) gave RR1NCOF, which was unreactive to SF4-KF. EtOCHO reacted with SF4-KF to give 35% EtOCF2H and 20% EtOCF3.
IT 683-81-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of, with sulfur tetrafluoride, in presence of potassium fluoride)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:449397 CAPLUS
DOCUMENT NUMBER: 97:49397
TITLE: Growth inhibition of a prostate tumor by α-difluoromethylornithine and by cyclophosphamide
AUTHOR(S): Heston, Warren D. W.; Kadmon, Dov; Fair, William R.
CORPORATE SOURCE: Sch. Med., Washington Univ., St. Louis, MO, 63110, USA
SOURCE: Cancer Letters (Shannon, Ireland) (1982), 16(1), 71-9
CODEN: CALEDQ; ISSN: 0304-3835
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effects of the ornithine decarboxylase suicide substrate difluoromethylornithine (DFMO) [82435-33-4] and cyclophosphamide [50-18-0] individually and in combination on the growth of the R3327MAT-Lu prostate derived tumor were determined DFMO decreased the growth rate and resulted in 75% reduction in DNA content compared to the control group. Cyclophosphamide produced a greater inhibition of growth and resulted in a 96% reduction in DNA content relative to the control. DFMO in combination with cyclophosphamide provided no greater inhibition of tumor growth than that of cyclophosphamide as a single agent. Further, in the schedule used in this exptl. protocol, the toxicity to the host of the drug combination was additive.
IT 82435-33-4
RL: BIOL (Biological study)
(neoplasm inhibition by cyclophosphamide and, DNA in relation to)
RN 82435-33-4 CAPLUS
CN Ornithine, N2-(difluoromethyl)- (9CI) (CA INDEX NAME)



L16 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:34405 CAPLUS
DOCUMENT NUMBER: 96:34405
TITLE: α-Fluoroalkylamines as a new source of unhydrated fluoride ion. 3. Fluorine-19 NMR spectra of perfluorocarbanions generated with N,N,N',N'-tetramethylformamidinium bifluoride
AUTHOR(S): Delyagina, N. I.; Igumnov, S. M.; Snegirev, V. F.; Knunyants, I. L.
CORPORATE SOURCE: Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (10), 2238-43
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 96:34405
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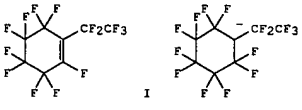
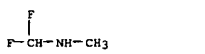


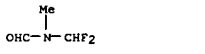
AB The reaction of [(Me2N)2CH]+ HF2- with (CF3)2C:CF2, (CF3)2C:CFCF2CF3, CF3CF2CF2C(CF3):CFCF2CF3, and I gave (CF3)3C-, (CF3)2C-CF2CF2CF3, (CF3CF2CF2)2C-CF3, and II, resp. The 19F NMR spectra of these carbanions were recorded. The carbanions were stable at low temps.
IT 683-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylamine)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:480015 CAPLUS
DOCUMENT NUMBER: 95:80015
TITLE: α-Fluoroalkylamines as a new source of unhydrated fluoride ion. 2. α,α-Difluorotrimethylamine
AUTHOR(S): Knunyants, I. L.; Delyagina, N. I.; Igumnov, S. M.
CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (4), 860-3
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 95:80015
AB Me2N+:CHF F- (I) reacted with (CF3)2C:CO, CF3NCO and (CF3)2C:CF2 (II) to give 83% (CF3)2C:CHNMe2, 91.0% CF3N:CHNMe2 and 35.0% Me2NCHFC(CF3)3, resp.
I also reacted with II and (CF3)2CO via a carbenoid mechanism to give 57.0% Me2NCF2CF:C(CF3)2 (III) and 40.0% 4-(dimethylamino)-2,2,5,5-tetrakis(trifluoromethyl)-1,3-dioxolane (IV). Deamination of IV with concentrated H2SO4 yielded 50% 2,2,5,5-tetrakis(trifluoromethyl)-1,3-dioxolan-4-one. Hydrolysis of II gave (CF3)2C:CFCONMe2 quant.
IT 683-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with perfluoroisobutylene, -acetone and -ketene and with tri-Me isocyanate)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:442254 CAPLUS
DOCUMENT NUMBER: 95:42254
TITLE: Preparation and study of difluoromethyl-substituted amines
AUTHOR(S): Allenstein, E.; Schrempf, G.
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1981), 474, 7-17
CODEN: ZAACAB; ISSN: 0044-2313
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 95:42254
AB Fluorinating RN(CHCl2)2 (R = Me, Et) and N(CHCl2)3 with SbF3 gave RN(CHF2)2 and N(CHF2)3, resp. Under certain conditions, MeN(CHO)2 with COF2 gave the known MeN(CHO)CHF2. RN(CHF2)2 and N(CHF2)3 are mols. with covalent C-F bonds. Treating MeN(CHF2)2 with SbF5 or BF3 cleaved a F-ion from a CHF2 group to give [MeN(CHF2):CHF]+ X- (X = SbF6 or BF4).
IT 78209-76-4P 78209-77-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78209-76-4 CAPLUS
CN Methanamine, 1,1-difluoro-N-methyl- (9CI) (CA INDEX NAME)

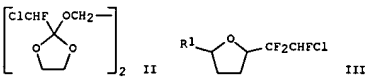


RN 78209-77-5 CAPLUS
CN Formamide, N-(difluoromethyl)-N-methyl- (9CI) (CA INDEX NAME)



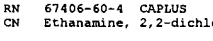
L16 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:567579 CAPLUS
DOCUMENT NUMBER: 93:167579
TITLE: Chemistry of organic fluorine compounds. XXI. Transformation of chlorofluoroethyldiethylamines to N,N-diethyldifluoroacetamide
AUTHOR(S): Liska, Frantisek; Hampl, Frantisek; Dedek, Vaclav
CORPORATE SOURCE: Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1980), 45(3), 740-5
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:167579
AB Differences in reactivity in nucleophilic substitution with F- were investigated in compds. containing CHCl2 and CHClF groups. Thus, hydrolysis of CHClFCF2NEt2 and CHCl2CF2NEt2 in the presence of Et3N gave, resp., CHClFCONEt2 (I) and CHCl2CONEt2 (II), which were fluorinated by HF. I readily yielded CHF2CONEt2 as the sole product, whereas II gave, by a markedly slower transformation, as the main product CHF2CONEt2 accompanied by <1% I, suggesting a weaker reactivity of the C-Cl bond in the CHCl2 group compared with CHClF.
IT 67406-60-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis-fluorination of)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)

L16 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:54416 CAPLUS
DOCUMENT NUMBER: 90:54416
TITLE: Chemistry of organic fluorine compounds. Part XIX. Reactions of fluoroalkanols and fluoroalkanediols with fluoroalkyl amines
AUTHOR(S): Dedek, Vaclav; Liska, Frantisek; Cvak, Ladislav
CORPORATE SOURCE: Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1978), 43(10), 2649-55
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

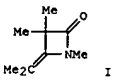


AB Fluoroalkylamines XCHClCF2NEt2 [X = F (I), Cl] mainly replace the OH group in ClCHFCF2CHMeCH2OH by F or Cl. HOCH2CH2OH decomps. I to give the orthoester II. The 1,4-butanediols ClCHFCF2CH(OH)(CH2)2CH(OH)R1 (R1 = H, CF2CHFCl) undergo dehydration to the tetrahydrofurans III.
IT 67406-60-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with fluoroalkanols)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)

L16 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:507949 CAPLUS
DOCUMENT NUMBER: 89:107949
TITLE: Chemistry of organic fluorine compounds; Part XVIII. Reaction of fluoroalkanols with fluoroalkylamines
AUTHOR(S): Dedek, Vaclav; Liska, Frantisek; Cvak, Ladislav
CORPORATE SOURCE: Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1978), 43(4), 985-97
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cl2CHCF2NEt2 (I) was prepared in 66% yield from Cl2C:CF2 and Et2NH. The reaction of I with BuOH, RCHFCF2CHR1OH (R = F, R1 = H; R = Cl, R1 = H, Me), and FClCHCF2CMe2OH gave BuF (in 75% yield), RCHFCF2CHR1OCF(NEt2)CHCl2 (II), and FClCHCF2CMe:CH2, resp. Hydrolysis of II led to RCHFCF2CHR1OCOCHCl2, and its decomposition above 150° to a mixture of RCHFCF2CHFR1 and RCHFCF2CHClR1 (mol ratio 3:1) and to Cl2CHCONEt2. The decompns. of fluorinating agents I and FClCHCF2NEt2 (III) at 100° in Pt and glass vessels were followed and the products were identified. Reactions of III with alcs. were adversely affected by their decomposition products and by glass.
IT 67406-60-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and reaction with fluoroalkanols)
RN 67406-60-4 CAPLUS
CN Ethanamine, 2,2-dichloro-N,N-diethyl-1,1-difluoro- (9CI) (CA INDEX NAME)



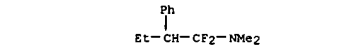
L16 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:104640 CAPLUS
DOCUMENT NUMBER: 88:104640
TITLE: Reactivity and synthetic potential of α-fluoro- and α-iodoenamines
AUTHOR(S): Colens, Alain; Ghosez, Leon
CORPORATE SOURCE: Lab. Chim. Synth., Univ. Louvain, Louvain, Belg.
SOURCE: Nouveau Journal de Chimie (1977), 1(5), 371-2
CODEN: NJCHD4; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:104640
GI



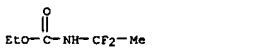
I

AB The nucleophilic character of α-fluoroenamines and the electrophilic character of α-iodoenamines was shown. E.g., Me2C:CFNMe2 reacted with Me2C:ClNMe2 in HCCl3 at 20° to give, after hydrolysis, the β-lactam I.
IT 65560-31-8P 65560-32-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65560-31-8 CAPLUS
CN 1-Propanamine, 1,1-difluoro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)

RN 65560-32-9 CAPLUS
CN Benzeneethanamine, β-ethyl-α,α-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



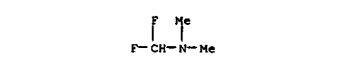
L16 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:576795 CAPLUS
DOCUMENT NUMBER: 85:176795
TITLE: Addition of carbonyl fluoride to aliphatic nitriles: formation of α,α-difluoroalkyl isocyanates
AUTHOR(S): Clifford, Alan F.; Thompson, James Wood
CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst., Blacksburg, VA, USA
SOURCE: Inorg. Nucl. Chem. - Herbert H. Hyman Mem. Vol. (1976)
, 37-43. Editor(s): Katz, Joseph J.; Sheft, Irving. Pergamon: Oxford, Engl.
CODEN: 33TZAU
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Carbonyl fluoride will add to alkane- and perfluoroalkanenitriles and alkanedinitriles in anhydrous acids to form the corresponding α,α-difluoroalkyl isocyanate, perfluoroalkyl isocyanate, or α,α,ω,ω,-tetrafluoro-α,ω-diisocyanatoalkane. With MeCN the reaction proceeded slowly in anhydrous HF
or in the presence of anhydrous HCl in C6H6 to give MeCF2NCO. The addition
reaction proceeded more rapidly with EtCN and less rapidly with F3CCN than
with MeCN. NCCH2 yielded F3CNCO and cyanuric acid. Adiponitrile produced
1,6-diisocyanato-1,1,6,6-tetrafluorohexane and 1-isocyanato-5-cyano-1,1-difluoropentane.
IT 60905-24-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60905-24-0 CAPLUS
CN Carbamic acid, (1,1-difluoroethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L16 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:19213 CAPLUS
DOCUMENT NUMBER: 64:19213
ORIGINAL REFERENCE NO.: 64:3501h,3502a-c
TITLE: Substituted acetonitriles
INVENTOR(S): Brown, Morton
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3214428		19651026	US 1961-100531	19610404

AB (R2N)2CHCN were prepared by reaction of α-dimethylamino-α-methoxyacetonitrile (I) with secondary aliphatic amines. A mixture of 146
parts HCONMe2 and 33 parts COF2 was allowed to stand at 25° for 21 hrs. in a pressure vessel at autogenous pressure to give 63% 1,1-difluorotrimethylamine (II), b. 47-51.5°. To a mixture of 486 parts anhydrous NaOMe in 1500 parts Et2O at 0° under N was added during 1 hr. 410 parts II to give 73% dimethylformamide dimethyl acetal (III), b. 101-2°, n25D 1.3957. To a solution of 35 parts HCN in 200 parts anhydrous Et2O at 0° was added during 0.5 hrs. 76 parts III. The mixture kept at 25° for 16 hrs. gave 93% I, b40 70-2°, n25D 1.4110. To 11.4 parts I in 50 parts C6H6, was added 14.2 parts pyrrolidine and the mixture refluxed 1 hr. with evolution of Me2NH. C6H6-MeOH azeotrope was slowly distilled and 68% α,α-di(pyrrolidino)acetonitrile (IV). b0.5 109-111°, n25D 1.4838, was isolated by distillation Similarly prepared were 65% 1,3-dimethyl-2-cyano-1,3-diazacyclohexane, m. 42-3°, 61% α,α-bis(dipropylamino)acetonitrile, b4.5 115-18°, n25D 1.4460, 65% 1,3-diethyl-2-cyanoimidazolidine, b42 130-3°, n25D 1.4532, 60%, α,α bis, N-methyl-cyclohexylamino)acetonitrile, b0.5 79°, n25D 1.4727, and α,α-di(piperidino)acetonitrile (V), b3.5 138-9°, n25D 1.4936. A solution of 25 parts α-collidine and 3 parts IV was heated at 175° for 24 hrs. under N with evolution of HCN to give 73% tetra(pyrrolidino)ethylene, m. 94-5°. V was heated at 250° and evolved HCN to give tetra(piperidino)ethylene, m. 59-61°. The compds. are useful as water scavengers in organic systems. The tetraminoethylenes are useful as
antioxidants and as chemical light sources since they chemiluminesce when exposed to air.
IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

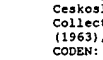


L16 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:474793 CAPLUS
DOCUMENT NUMBER: 59:74793
ORIGINAL REFERENCE NO.: 59:13802h,13803a-b
TITLE: Synthetic reactions of dimethylformamide. XIX. Preparation of α-difluorotrimethylamine and some of its reactions
AUTHOR(S): Arnold, Z.
CORPORATE SOURCE: Ceskoslov. Akad. Ved, Prague
SOURCE: Collection of Czechoslovak Chemical Communications (1963), 28(8), 2047-51
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
AB COCl2 was passed through 73.1 g. HCONMe2 in 300 ml. CHCl3 in an icewater bath as long as CO2 was formed, the solution transferred to a polythene flask, stirred, and heated in a boiling water bath in vacuo to remove excess COCl2 and solvent. The flask was placed into an ice-salt freezing mixture and dry HF passed in with intermittent shaking until the increase in
weight was about 300 g. Next day, excess HF was evaporated by heating to 65° the material transferred to an Fe vessel, and residual HF removed at 120°. The residue was distilled in vacuo and the obtained intermediate trihydrofluoride, C3H10F6N (15.5 g.), b30 80°, was distilled over anhydrous KF to give 7.4 g α,α-difluorotrimethylamine (I), b. 48-50°, n2D0 1.3315. Similarly, 3 g. PhCONMe2 added under ice-cooling to a solution of 6 g. COCl2 in 20 mh CHCl3 and the solution treated
as above gave 2.1 g. α,α-difluorobenzyldimethylamine, b. 70-90°, n2D0 1.4738. Solns. of I in organic solvents gave with BF3 etherate a crystalline hygroscopic precipitate, C3H7BF5N, m. 47-51°, ν 1670,
1737, 8071, and 3141 cm.-1 I (3.1 g.) treated with stirring and cooling with 1.2 g. BzOH and the mixture kept at room temperature with stirring 1 hr. gave
1.1 g. BzF, b. 50-5°, n20D0 1.4968, 3.1 g. I heated with 1.06 g. BzH 3 hrs. at 85° in an Fe tube yielded 0.95 g. α,α-difluorotoluene, b. 145-50°, n2D0 1.4572. BzNH2 kept with a solution of I in dioxane 20 min. at -5° gave 81.5% BzCN. When a stirred solution of 2',3'-O-isopropylidene-6-azauridine in HCONMe2 was
treated with ice-cooling with I in HCONMe2 and the product analyzed by means of paper chromatography, only a spot corresponding to the formate could be detected.
IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

L16 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:474792 CAPLUS
DOCUMENT NUMBER: 59:74792
ORIGINAL REFERENCE NO.: 59:13802d-h
TITLE: Synthetic reactions of dimethylformamide. XVIII. Reactivity of methyl groups in polymethinium salts
AUTHOR(S): Arnold, Z.; Holy, A.
CORPORATE SOURCE: Ceskoslov. Akad. Ved, Prague
SOURCE: Collection of Czechoslovak Chemical Communications (1963), 28(8), 2040-6
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 59:74792

AB cf. CA 59, 5055c. The reaction of acetals, Me2NCH(OR)2, with polymethinium salts leaves the fundamental system untouched and the reaction takes place only on Me groups located in position 1 and 3 of the polymethinium chain. The 2-Me derivs. do not react under similar conditions. A mixture of 20 g. CH2Ac2 and a 1.2M solution of NHMe2 in 250 ml. C6H6 was heated in an autoclave 4 hrs. at 100° evaporated, and the residue fractionated to give 12.6 g. Me2NCMe:CHAc, b12 125°, m. 46-7° (Et2O). BzCH2Ac yielded analogously 35.5% Me2NCMe: CHBz, m. 68-9° (cyclohexane), b0.1 150-5°. The amine (0.05 mole) was heated with 0.05 mole freshly distilled Me2SO4 4 hrs. at 80-90° under exclusion of moisture, the mixture cooled, dissolved in 20 ml. dry CHCl3, the solution treated with stirring and cooling to -40° with 0.075 mole R2NH in 60 ml. C6H6, the mixture stirred 1 hr. at room temperature, the solvent evaporated in vacuo, the residue dissolved in 20 ml. H2O, and treated with 10.5 g. NaClO4 in 20 ml. water to give the following trimethinium salts, [Me2N: CR1CR2: CR3NR42] +ClO4- (I) (R1, R2, R3, R4, % yield, and m.p. given): H, Me, H, Me (Ia), 60, 92-3°; Me, H, Me, Me, 64, 153-4°; Me, H, Ph, Me, 88, 112-13°; H, H, H, Et, 61, 94-5°; Me, H, H, Et, 52, 98-9°. Heating a suspension of 0.005 mole I in 5 ml. HCONMe2 with 0.015 mole Me2NCH(OMe)2 or Me2NCH(OEt)2 4 hrs. at 80°, evaporating the mixture in vacuo to dryness, treating the residue with 20 ml. H2O, and working up as above gave the following [Me2N:CHCH:C(NMe2)CH:CRNMe2+ClO4- (II) (R, % yield, and m.p. given): H, 65, 188-9°; Ph, 88.4, 138-9°; Me, 35.2, 2723°. Ia failed to react under the same conditions. II (0.004 mole) was heated 4 hrs. at 100° in a solution of 0.01 mole NH4Cl in 10 ml. H2O, the mixture made alkaline to pH 10 with Na2CO3, and extracted with CHCl3 to give cyclized products, e.g. 78.2% γ-dimethylaminopyridine, m. 114° (cyclohexane), and 49.4% α-phenyl-γdimethylaminopyridine, m. 83-4° (petr. ether). [Me2NCH:CHCMe: CHCH: NMe2] +ClO4- (5.4 g.) was refluxed with 0.12 mole [Me2N: CHCl] +Cl- in 60 ml. CHCl3 2.5 hrs. with exclusion of moisture, CHCl3 evaporated in vacuo, and the residue treated with 50 g. ice and 8.40 g. crystalline NaClO4 to give 12.4 g. yellow product, m. 300°, apparently [Me2NCH:C(CH: NMe2)C(:CHCH: NMe2)C(:CHNMe2)CH: NMe2]3+3ClO4-, which yielded on double cyclization with NH4Cl as above 80% 4-formyl-2,7-naphthyridine, m. 215-16° (CCl4). The relationship between reactivity of alkyl groups and their position on a polymethinium chain is discussed.

L16 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

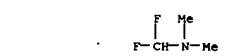


L16 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:469068 CAPLUS
DOCUMENT NUMBER: 59:69068
ORIGINAL REFERENCE NO.: 59:12764g-h,12765a
TITLE: Actals and ketals of N,N-disubstituted carboxamides
INVENTOR(S): Brown, Morton
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3092637		19630604	US 1961-91571	19630227

AB Tertiary amines are prepared by reaction between an alkali metal or alkaline earth metal salt of an alc. or phenol and a 1,1-dihalo-substituted tertiary amine (I). I are in turn prepared by treating the corresponding N,N-disubstituted amide with a halogenating agent, e.g. COF2, SOCl2, COCl2, SF4. HCONMe2 146 and COF2 33 parts kept 21 hrs. at 25° in a pressure vessel, and the mixture distilled, gave 30 parts HCF2NMe2 (II), b. 47-51.5°. II 410 added dropwise to NaOMe 486 in Et2O 1500 parts at 0° under N, and the mixture kept 1 hr. at room temperature and distilled, gave 374 parts HC(OMe)2NMe2, b. 101-2°, n25D 1.3957. Similarly, II and NaOEt gave HC(OEt)2NMe2, b. 131.0-2.5°, n25D 1.4010; PhCF2NMe2 and NaOMe gave PhC(OMe)2NMe2, b5 65-8°, n25D 1.5045; (Me2N)2CF2 (b. 101-3°, from (Me2N)2CO and COF2) and NaOMe gave (Me2N)2C(OMe)2, b44 69-70°, n25D 1.4242; MeCCl2NMe2 (solid, from AcNMe2 and COCl2) and NaOMe gave MeC(OMe)2NMe2, b. 118-20°, n25D 1.4047-52; N-dichloromethylpyrrolidine [from N-formylpyrrolidine and (COCl)2] and NaOMe gave N-dimethoxymethylpyrrolidine, b26 67-9°, n25D 1.4350; II and Me2C(CH2ONa)2 gave 2-dimethylamino-5,5-dimethyl-1,3-dioxane, b. 178-80°, n25D 1.4348; N-cyclohexyl- N -methyldifluoromethylamine (b23 65-8°, from N-cyclohexyl-N-methylformamide and COF2) and NaOMe gave N-cyclohexyl-N-methyldimethoxymethylamine, b24 115-16°, n25D 1.4378. The amide acetals and ketals are useful as scavengers for H2O and other active H-containing materials.

IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L16 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:66176 CAPLUS
DOCUMENT NUMBER: 58:66176
ORIGINAL REFERENCE NO.: 58:11243b-d
TITLE: The chemistry of xylylenes. XVIII. The gas phase synthesis of α,α'-bis(trichloromethyl)-p-xylene via coaxial pyrolysis of p-xylene and chloroform
AUTHOR(S): Errede, L. A.; Cassidy, J. P.
CORPORATE SOURCE: Minnesota Mining and Manuf. Co., St. Paul
SOURCE: Journal of Organic Chemistry (1963), 28, 1059-63
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB cf. CA 58, 8875b. Fast flowing streams of p-xylene and chloroform were pyrolyzed in separate concentric tubes. The resulting pyrolyzates were allowed to mix at a predetd. point downstream where coupling of the chlorocarbon and hydrocarbon radicals occurred to produce a mixture of products. The composition of reactive species in the resp. gas streams changed with distance away from the point of generation via pyrolysis. Hence, the product distribution changed accordingly with the blend point. Thus, p-methylbenzyl chloride and β,β-dichloro-p-methylstyrene were isolated as major products when the two streams were made to blend within the pyrolysis zone, whereas p-methylbenzyl chloride and α,α'-bis(trichloromethyl)-p-xylene (I) were isolated as major products when the pyrolyzates were allowed to blend five inches beyond the pyrolysis zone.

IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)
RN 683-81-8 CAPLUS
CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

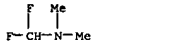
L16 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:66175 CAPLUS
DOCUMENT NUMBER: 58:66175
ORIGINAL REFERENCE NO.: 58:11243a-b
TITLE: Chemistry of carbonyl fluoride. I. Fluorination of organic compounds
AUTHOR(S): Fawcett, F. S.; Tullock, C. W.; Coffman, D. D.
CORPORATE SOURCE: E. I. du Pont de Nemours Co., Wilmington, DE
SOURCE: Journal of the American Chemical Society (1962), 84, 4275-85
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:66175

AB Carbonyl fluoride reacts with carbonyl compds. such as cyclohexanone, benzaldehyde, and benzophenone to give the gem-difluorides, while HCONMe2 yields α,α-difluorotrimethylamine. Metal fluoride-catalyzed addition at the ethylenic bond in perfluoro olefins forms perfluoroacyl fluorides, while the C-N unsatd, compds. CF3N: CF2, PhNCO, and CF3CN give, resp., (CF3)2NCOF, PhN(COF)2, and CF3CF2NCO. The exptl. technique, infrared and nuclear magnetic resonance spectra are given.

IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)

RN 683-81-8 CAPLUS

CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L16 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:39842 CAPLUS
DOCUMENT NUMBER: 58:39842
ORIGINAL REFERENCE NO.: 58:6752f-h
TITLE: Phenyl o-propargyloxybenzoate
INVENTOR(S): Sterling, George B.; Pawloski, Chester E.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: 1 p.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3061631		19621030	US 1961-97721	19610323

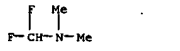
GI For diagram(s), see printed CA Issue.

AB Compds. of the general formula I were used to control the growth of wild oats and millet. 4-(2-HOC6H4CO2)C6H4CMe3 (204 g.), 125 g. HC.tplbond.CCH2Br, and 144 gr. K2CO3 were refluxed in 500 ml. Me2CO, 80 hrs., the mixture filtered, and the filtrate fractionally distilled in vacuo to give I, R = 4-tert-Bu, d25 1.076, n25D 1.5375. Similarly prepared were I (R given): H, d25 1.169, n25D 1.5769; 2-Me; 4-C5H11; 3-Me; 2-Bu; 4-Et.

IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)

RN 683-81-8 CAPLUS

CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L16 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:39841 CAPLUS
DOCUMENT NUMBER: 58:39841
ORIGINAL REFERENCE NO.: 58:6752d-f
TITLE: Fluorinated organic compounds
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 11 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

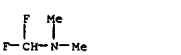
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 909364		19621031	GB 1960-38526	19601109
US 3213062		19651019	US 1959-852939	19591116
PRIORITY APPLN. INFO.:			US	19591116

AB The title compds. can be used as chemical intermediates. Cyclohexanone 40, COF2 65, and HCONMe2 4-5 parts are placed in a reactor containing N, the reactor is closed, the mixture heated at 50° 12 hrs. under autogenous pressure, cooled, the volatile materials are removed, and the remaining liquid is distilled to give 1-fluorocyclohexyl fluoroformate (I), b27 59-63°, 52 parts. I 17, hexane 30-5, and BF3-etherate 4.8 parts are heated at 45-7° 3 hrs., the mixture is cooled, the upper phase separated, agitated with powdered NaF, the NaF filtered off, the filtrate evaporated, and the residue distilled through a fractionating column to give 1,1-di-fluorocyclohexane, b. 101-7°, n25D 1.3900-1.3895, 5.6 parts. Similarly prepared are Ph2CF2, b15 100-1°, n25D 1.5360-1.5368; PhCHF2, b15 35-6°; 4-Me2NC6H4CHF2; (FCH2)2O; PhCF3 and BzF; F3C(CF2)2COF; F3C(CF2)6COF, b. 108-9°; FOC(CF2)3COF, b. 47-9°; FOC(CF2)2COF, b. 30-5°; 2-F3CC6H4COF and phthaloyl fluoride; Me(F2CH)NCOF and Me(HCO)NCOF; Me(MeCF2)NCOF, b. 97-100° and MeAcNCOF, b. 136-8°; F2CHNMe2, b. 47-51.5°; PhCF2NMe2, b. 63°; N-fluoroformyl-1,1-difluorohexamethyleneimine, b0-5. 50°; and Me2NCF2NMe2, b. 101-3°.

IT 683-81-8, Trimethylamine, 1,1-difluoro-
(preparation of)

RN 683-81-8 CAPLUS

CN Methanamine, 1,1-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



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L17 ANSWER 1 OF 1 CAOLD COPYRIGHT 2006 ACS on STN
AN CA53:12236a CAOLD
TI reaction of SF4 with carbonyl derivs.
AU Smith, William Channing
PA Du Pont de Nemours, E. I., & Co.
DT Patent

PATENT NO.	KIND	DATE
US 2859245		1958
DE 1080993		

IT 75-37-6 98-08-8 98-15-7 312-96-9 360-11-2 368-94-5
369-54-0 371-90-4 420-45-1 425-32-1 433-19-2 433-95-4
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FULL ESTIMATED COST	4.83	512.25

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